

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptasj11626

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'CAPLUS' AT 17:14:08 ON 17 APR 2007  
FILE 'CAPLUS' ENTERED AT 17:14:08 ON 17 APR 2007  
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	6.21	511.91
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.78	-5.46

=> d his

(FILE 'HOME' ENTERED AT 16:20:09 ON 17 APR 2007)

FILE 'REGISTRY' ENTERED AT 16:20:17 ON 17 APR 2007  
L1           STRUCTURE UPLOADED  
L2           0 S L1  
L3           STRUCTURE UPLOADED  
L4           1 S L3  
L5           35 S L3 SSS FULL  
              SAV TEM BRD565557/A L5

FILE 'CAPLUS' ENTERED AT 16:24:21 ON 17 APR 2007  
L6           6 S L5  
              SAV TEM ANS565557/A L6

FILE 'REGISTRY' ENTERED AT 16:48:34 ON 17 APR 2007  
L7           STRUCTURE UPLOADED  
L8           9 S L7  
L9           855 S L7 SSS FULL  
              SAV TEM BRI565557/A L9

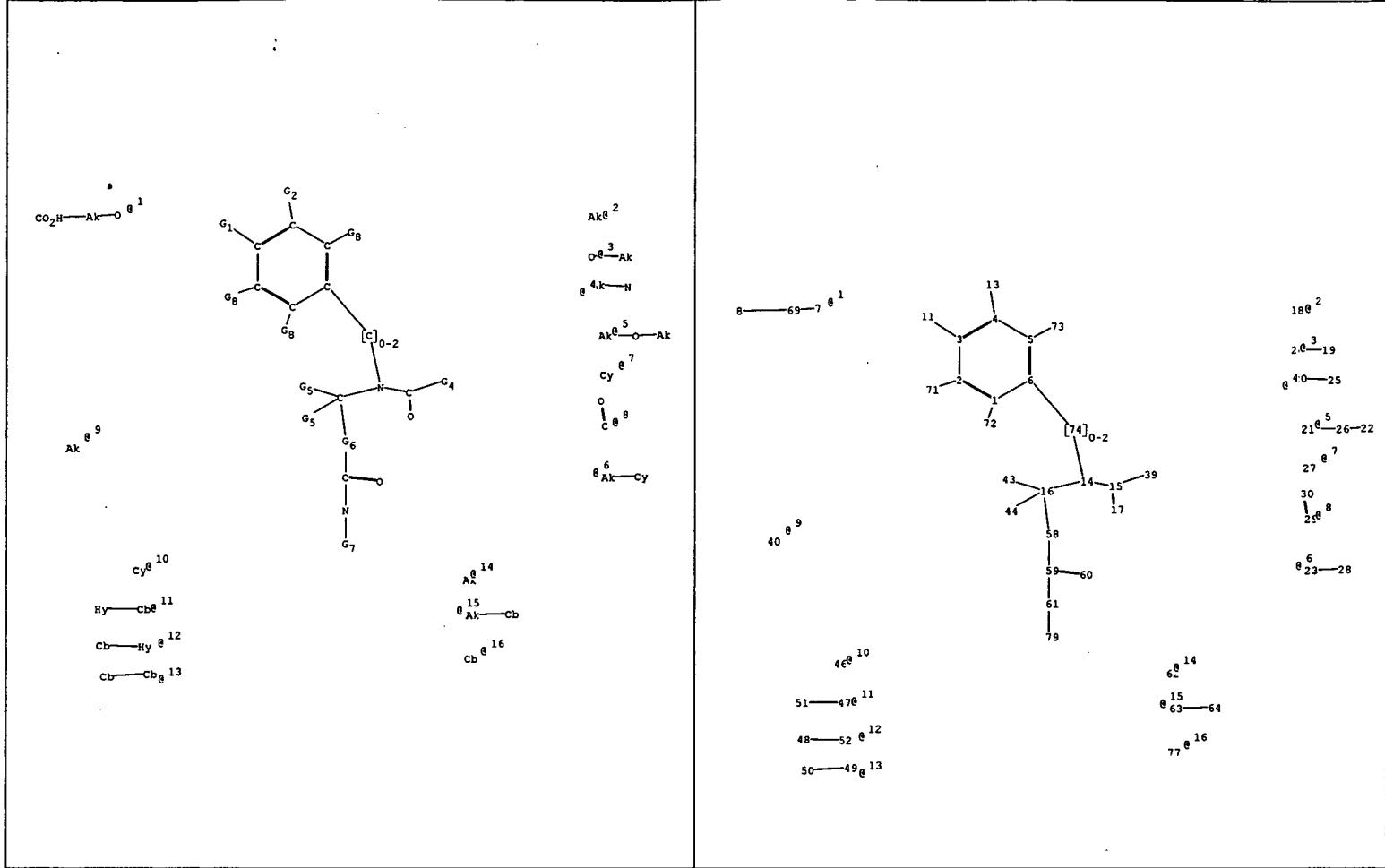
FILE 'STNGUIDE' ENTERED AT 16:49:43 ON 17 APR 2007

FILE 'REGISTRY' ENTERED AT 17:03:32 ON 17 APR 2007  
L10          STRUCTURE UPLOADED  
L11          STRUCTURE UPLOADED  
L12          STRUCTURE UPLOADED  
L13          28 S L10 SSS FULL SUB=L9  
              SAV TEM FIA565557/A L13  
L14          2 S L11 SSS FULL SUB=L9  
              SAV TEM FIB565557/A L14  
L15          1 S L12 SSS FULL SUB=L9  
              SAV TEM FIC565557/A L15

FILE 'CAPLUS' ENTERED AT 17:06:23 ON 17 APR 2007  
L16          4 S L13  
L17          1 S L14  
L18          1 S L15  
L19          0 S L17 NOT L16

L20

0 S L18 NOT L16



chain nodes :

7	8	11	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
29	30	39	40	43	44	46	47	48	49	50	51	52	58	59	60	61	62	63
64	69	71	72	73	74	77	79											

ring nodes :

1	2	3	4	5	6
---	---	---	---	---	---

chain bonds :

1-72	2-71	3-11	4-13	5-73	6-74	7-69	8-69	14-16	14-15	14-74	15-17
15-39	16-43	16-44	16-58	19-24	20-25	21-26	22-26	23-28	29-30	47-51	
48-52	49-50	58-59	59-60	59-61	61-79	63-64					

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6
-----	-----	-----	-----	-----	-----

exact/norm bonds :

1-72	2-71	3-11	4-13	5-73	7-69	8-69	14-16	14-15	14-74	15-17	15-39
16-43	16-44	16-58	19-24	20-25	21-26	22-26	23-28	29-30	47-51	48-52	
58-59	59-60	59-61	61-79	63-64							

exact bonds :

6-74	49-50
------	-------

normalized bonds :

1-2	1-6	2-3	3-4	4-5	5-6
-----	-----	-----	-----	-----	-----

isolated ring systems :

containing 1 :
----------------

G1:OH,CO2H, [\*1]

G2:OH,CO2H,H,CH3

G4:[\*2],[\*3],[\*4],[\*5],[\*6],[\*7],[\*8]

G5:H,[\*9]

G6:[\*10],[\*11],[\*12],[\*13]

G7:[\*14],[\*15],[\*16]

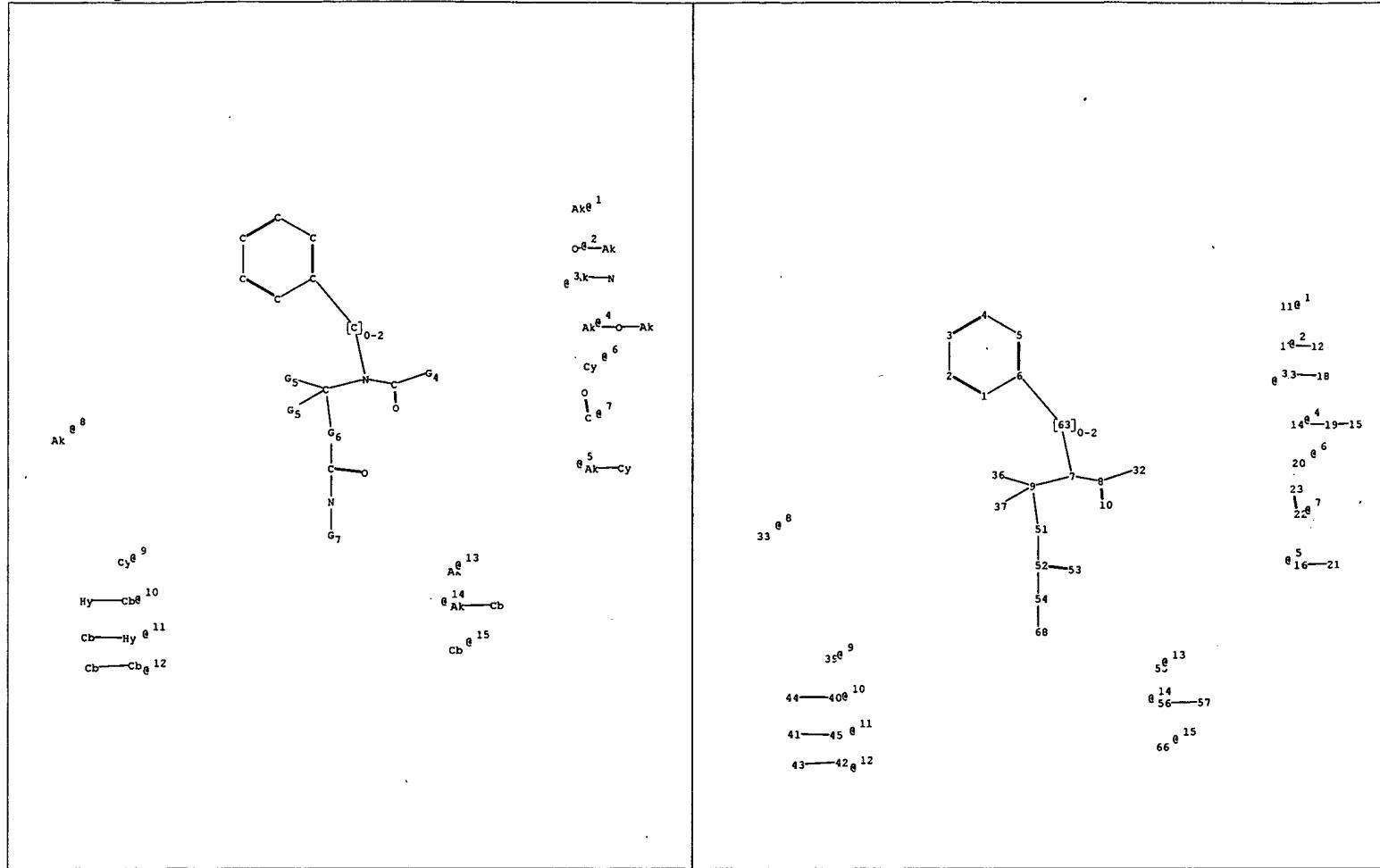
G8:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 11:CLASS  
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS  
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS  
27:Atom 28:Atom 29:CLASS 30:CLASS 39:CLASS 40:CLASS 43:CLASS  
44:CLASS 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom  
58:CLASS 59:CLASS 60:CLASS 61:CLASS 62:CLASS 63:CLASS 64:Atom  
69:CLASS 71:CLASS 72:CLASS 73:CLASS 74:CLASS 77:Atom 79:CLASS

Generic attributes :

40: Saturation : Saturated  
47: Saturation : Unsaturated  
48: Saturation : Unsaturated  
49: Saturation : Unsaturated  
50: Saturation : Unsaturated  
51: Saturation : Unsaturated  
52: Saturation : Unsaturated  
64: Type of Ring System : Monocyclic  
69: Type of chain : Linear  
Saturation : Saturated



chain nodes :

7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	32	33	36
37	39	40	41	42	43	44	45	51	52	53	54	55	56	57	63	66	68		

ring nodes :

1 2 3 4 5 6

chain bonds :

6-63 7-9 7-8 7-63 8-10 8-32 9-36 9-37 9-51 12-17 13-18 14-19  
 15-19 16-21 22-23 40-44 41-45 42-43 51-52 52-53 52-54 54-68 56-57

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

7-9 7-8 7-63 8-10 8-32 9-36 9-37 9-51 12-17 13-18 14-19 15-19

16-21 22-23 40-44 41-45 51-52 52-53 52-54 54-68 56-57

exact bonds :

6-63 42-43

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

### isolated ring systems :

containing 1 :

G4: [\*1], [\*2], [\*3], [\*4], [\*5], [\*6], [\*7]

G5 : H, [\* 8 ]

G6: [\*9], [\*10], [\*11], [\*12]

G7: [\*13], [\*14], [\*15]

G8: H, CH<sub>3</sub>

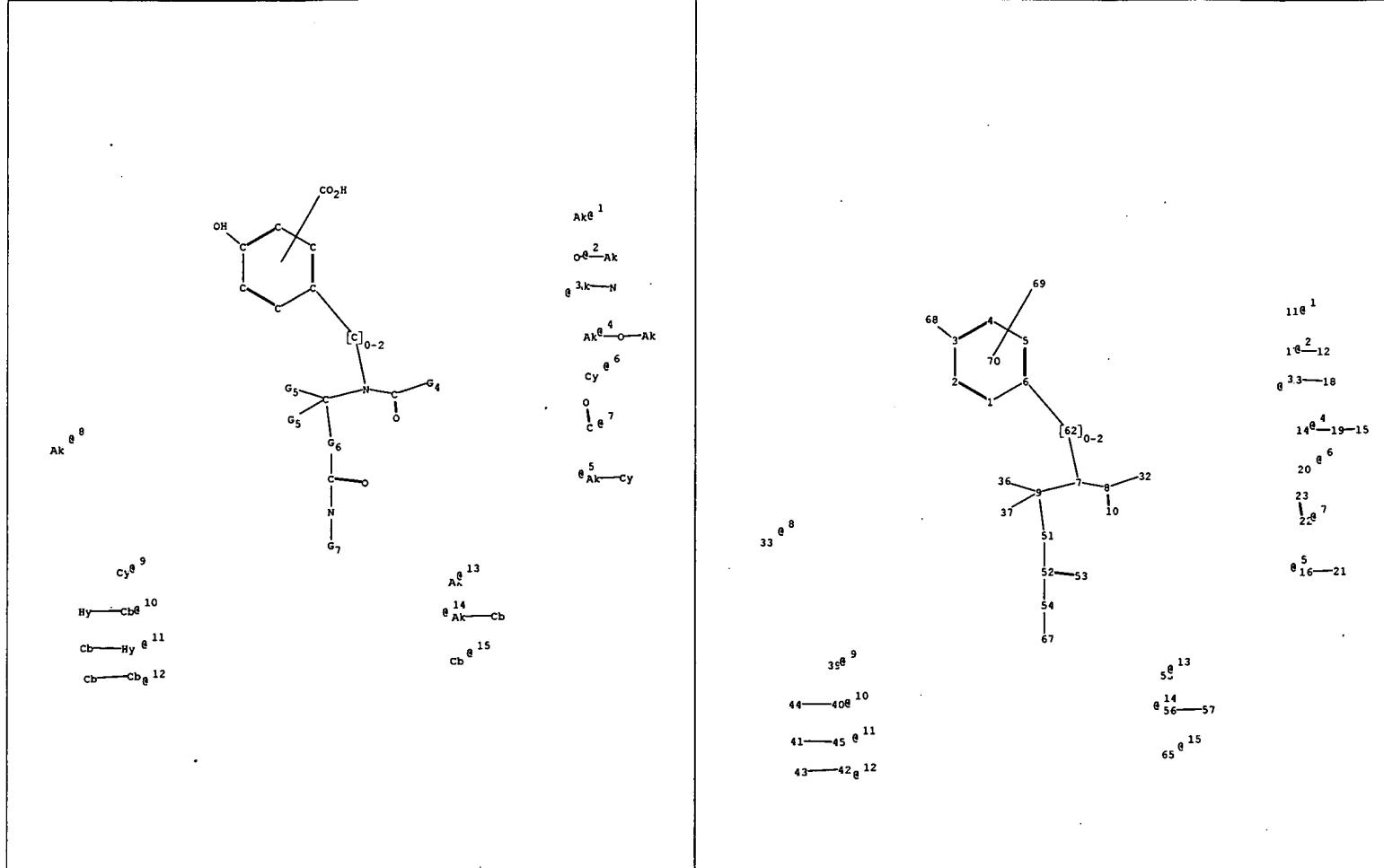
G9:0

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS  
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS  
17:CLASS 18:CLASS 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS  
32:CLASS 33:CLASS 36:CLASS 37:CLASS 39:Atom 40:Atom 41:Atom 42:Atom  
43:Atom 44:Atom 45:Atom 51:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS  
56:CLASS 57:Atom 63:CLASS 66:Atom 68:CLASS

Generic attributes :

33:  
Saturation : Saturated  
40:  
Saturation : Unsaturated  
41:  
Saturation : Unsaturated  
42:  
Saturation : Unsaturated  
43:  
Saturation : Unsaturated  
44:  
Saturation : Unsaturated  
45:  
Saturation : Unsaturated  
57:  
Type of Ring System : Monocyclic



chain nodes :

7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 32 33 36  
37 39 40 41 42 43 44 45 51 52 53 54 55 56 57 62 65 67 68  
69

ring nodes :

1 2 3 4 5 6

chain bonds :

3-68 6-62 7-9 7-8 7-62 8-10 8-32 9-36 9-37 9-51 12-17 13-18  
14-19 15-19 16-21 22-23 40-44 41-45 42-43 51-52 52-53 52-54 54-67  
56-57

ring bonds :

1-2    1-6    2-3    3-4    4-5    5-6

exact/norm bonds :

3-68	7-9	7-8	7-62	8-10	8-32	9-36	9-37	9-51	12-17	13-18	14-19
15-19	16-21	22-23	40-44	41-45	51-52	52-53	52-54	54-67	56-57		

exact bonds :

6-62 42-43

normalized bonds :

1-2 1-6 2-3

### isolated ring systems :

containing 1 :

G4: [-1], [-2], [-3], [-4], [-5], [-6], [-7]

85.11, [ 8 ]

G6: [^9], [^10], [^11], [^12]

G/: [\*13], [\*14], [\*15]

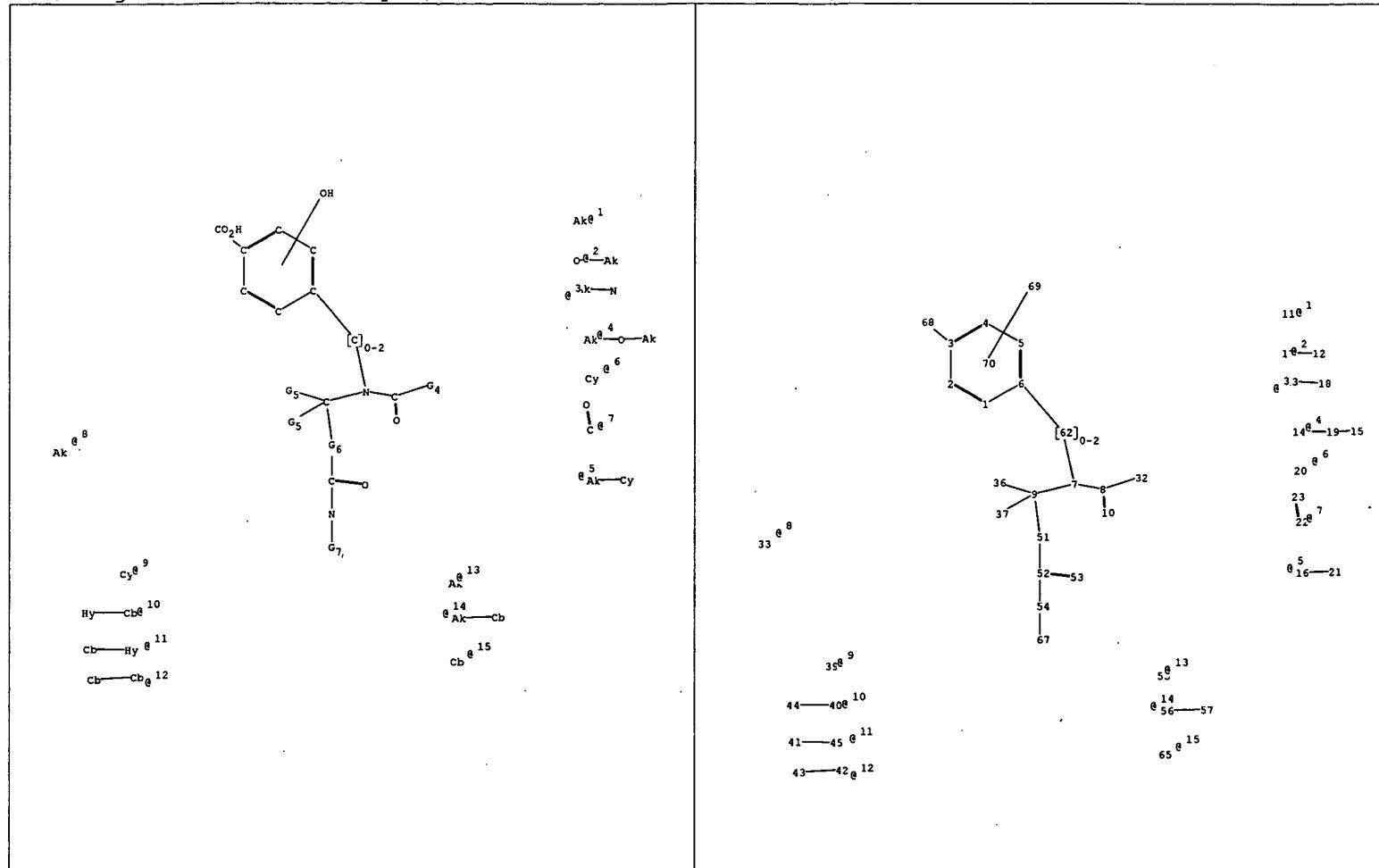
G8:H, CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS  
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS  
17:CLASS 18:CLASS 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS  
32:CLASS 33:CLASS 36:CLASS 37:CLASS 39:Atom 40:Atom 41:Atom 42:Atom  
43:Atom 44:Atom 45:Atom 51:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS  
56:CLASS 57:Atom 62:CLASS 65:Atom 67:CLASS 68:CLASS 69:CLASS 70:Atom

Generic attributes :

33:  
Saturation : Saturated  
40:  
Saturation : Unsaturated  
41:  
Saturation : Unsaturated  
42:  
Saturation : Unsaturated  
43:  
Saturation : Unsaturated  
44:  
Saturation : Unsaturated  
45:  
Saturation : Unsaturated  
57:  
Type of Ring System : Monocyclic



chain nodes :

7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 32 33 36  
37 39 40 41 42 43 44 45 51 52 53 54 55 56 57 62 65 67 68  
69

ring nodes :

1 2 3 4 5 6

chain bonds :

3-68 6-62 7-9 7-8 7-62 8-10 8-32 9-36 9-37 9-51 12-17 13-18  
14-19 15-19 16-21 22-23 40-44 41-45 42-43 51-52 52-53 52-54 54-67  
56-57

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

7-9 7-8 7-62 8-10 8-32 9-36 9-37 9-51 12-17 13-18 14-19 15-19  
 16-21 22-23 40-44 41-45 51-52 52-53 52-54 54-67 56-57

exact bonds :

3-68 6-62 42-43

normalized bonds :

1-2    1-6    2-3    3-4    4-5    5-6

## isolated ring systems

containing 1 :

G4: [\*1], [\*2], [\*3], [\*4], [\*5], [\*6], [\*7]

G5 : H, [\*8]

G6: [\*9], [\*10], [\*11], [\*12]

G7: [\*13], [\*14], [\*15]

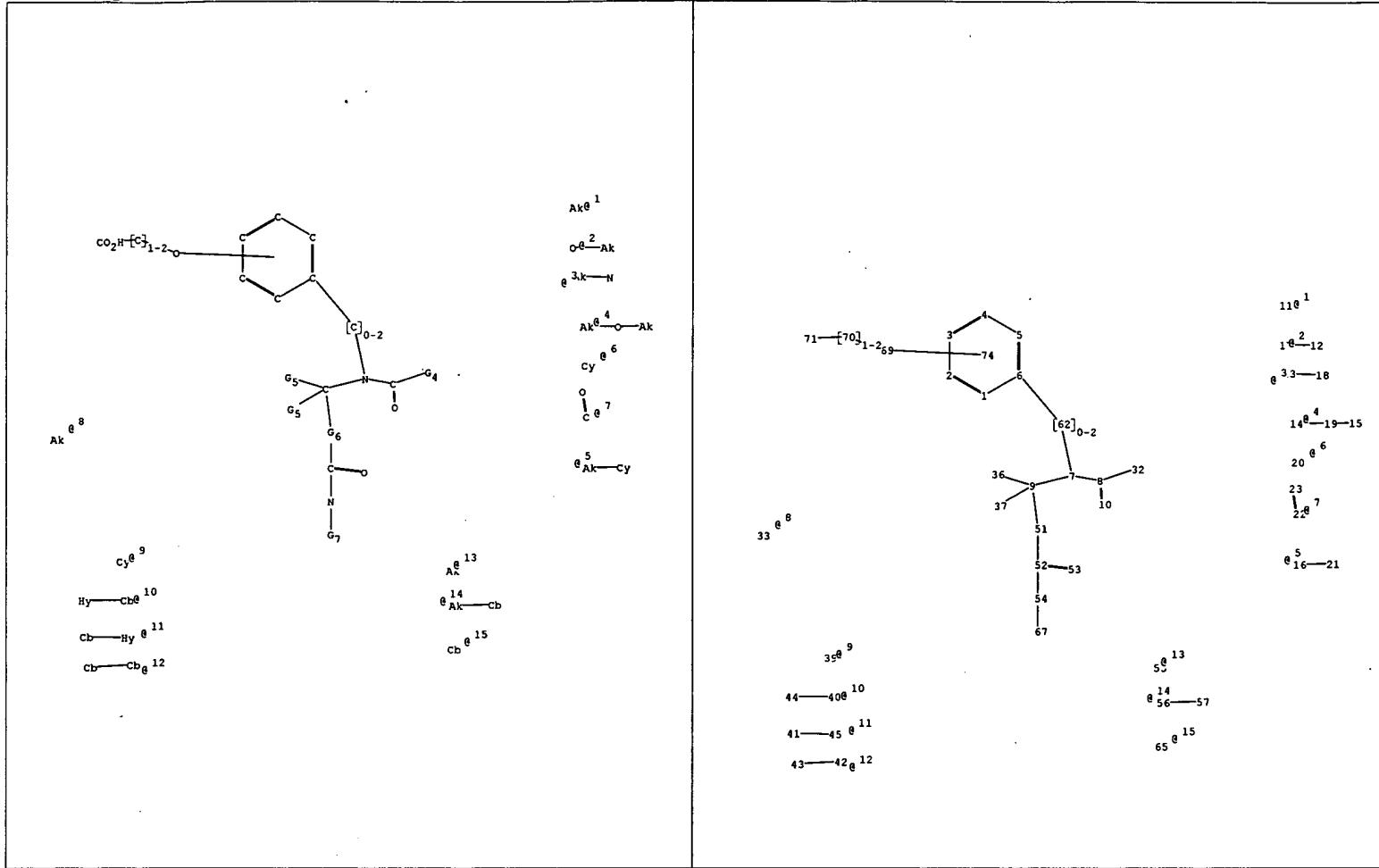
G8:H, CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS  
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS  
17:CLASS 18:CLASS 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS  
32:CLASS 33:CLASS 36:CLASS 37:CLASS 39:Atom 40:Atom 41:Atom 42:Atom  
43:Atom 44:Atom 45:Atom 51:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS  
56:CLASS 57:Atom 62:CLASS 65:Atom 67:CLASS 68:CLASS 69:CLASS 70:Atom

Generic attributes :

33:  
Saturation : Saturated  
40:  
Saturation : Unsaturated  
41:  
Saturation : Unsaturated  
42:  
Saturation : Unsaturated  
43:  
Saturation : Unsaturated  
44:  
Saturation : Unsaturated  
45:  
Saturation : Unsaturated  
57:  
Type of Ring System : Monocyclic



chain nodes :

7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	32	33	36
37	39	40	41	42	43	44	45	51	52	53	54	55	56	57	62	65	67	69	
70	71																		

ring nodes :

1	2	3	4	5	6
---	---	---	---	---	---

chain bonds :

6-62	7-9	7-8	7-62	8-10	8-32	9-36	9-37	9-51	12-17	13-18	14-19								
15-19	16-21	22-23	40-44	41-45	42-43	51-52	52-53	52-54	54-67	54-67	56-57	69-70	70-71						

ring bonds :

1-2	1-6	2-3	3-4	4-5	5-6
-----	-----	-----	-----	-----	-----

exact/norm bonds :

7-9	7-8	7-62	8-10	8-32	9-36	9-37	9-51	12-17	13-18	14-19	15-19								
16-21	22-23	40-44	41-45	51-52	52-53	52-54	54-67	56-57	56-57	69-70									

exact bonds :

6-62	42-43	70-71
------	-------	-------

normalized bonds :

1-2	1-6	2-3	3-4	4-5	5-6
-----	-----	-----	-----	-----	-----

isolated ring systems :

containing 1 :
----------------

G4: [\*1], [\*2], [\*3], [\*4], [\*5], [\*6], [\*7]

G5: H, [\*8]

G6: [\*9], [\*10], [\*11], [\*12]

G7: [\*13], [\*14], [\*15]

G8: H, CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS  
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS  
17:CLASS 18:CLASS 19:CLASS 20:Atom 21:Atom 22:CLASS 23:CLASS  
32:CLASS 33:CLASS 36:CLASS 37:CLASS 39:Atom 40:Atom 41:Atom 42:Atom  
43:Atom 44:Atom 45:Atom 51:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS  
56:CLASS 57:Atom 62:CLASS 65:Atom 67:CLASS 69:CLASS 70:CLASS  
71:CLASS 74:Atom

Generic attributes :

33:  
Saturation : Saturated  
40:  
Saturation : Unsaturated  
41:  
Saturation : Unsaturated  
42:  
Saturation : Unsaturated  
43:  
Saturation : Unsaturated  
44:  
Saturation : Unsaturated  
45:  
Saturation : Unsaturated  
57:  
Type of Ring System : Monocyclic

FILE 'HOME' ENTERED AT 16:20:09 ON 17 APR 2007

=> fil reg		SINCE FILE	TOTAL
COST IN U.S. DOLLARS		ENTRY	SESSION
FULL ESTIMATED COST		0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:20:17 ON 17 APR 2007  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 16 APR 2007 HIGHEST RN 930395-50-9  
DICTIONARY FILE UPDATES: 16 APR 2007 HIGHEST RN 930395-50-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

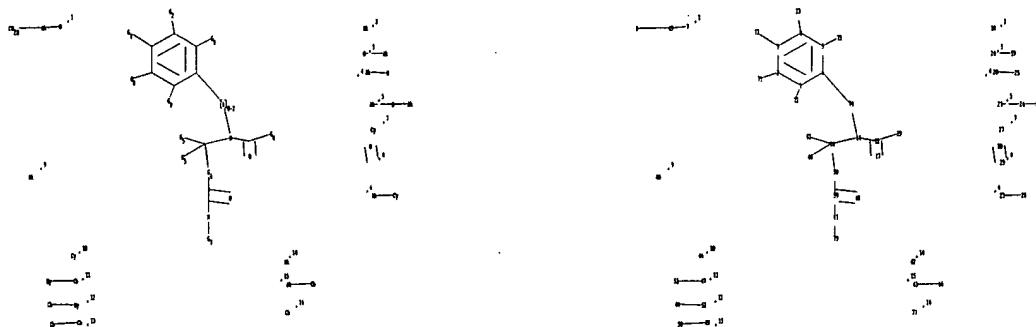
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10565557-broad.str



chain nodes :

7	8	11	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
39	40	43	44	46	47	48	49	50	51	52	58	59	60	61	62	63	64	69	71	72
73	74	77	79																	

ring nodes :

1 2 3 4 5 6

chain bonds :

1-72	2-71	3-11	4-13	5-73	6-74	7-69	8-69	14-16	14-15	14-74	15-17	15-39
16-43	16-44	16-58	19-24	20-25	21-26	22-26	23-28	29-30	47-51	48-52	49-50	58-59
59-60												

59-61 61-79 63-64

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-72	2-71	3-11	4-13	5-73	6-74	7-69	8-69	14-16	14-15	14-74	15-17	15-39
16-43	16-44	16-58	19-24	20-25	21-26	22-26	23-28	29-30	47-51	48-52	58-59	59-60
61-79	63-64											

exact bonds :

49-50

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:OH,CO2H, [\*1]

G2:OH,CO2H,CH3

G4:[\*2],[\*3],[\*4],[\*5],[\*6],[\*7],[\*8]

G5:H,[\*9]

G6:[\*10],[\*11],[\*12],[\*13]

G7:[\*14],[\*15],[\*16]

G8:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 11:CLASS 13:CLASS  
14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS  
22:CLASS 23:CLASS  
24:CLASS 25:CLASS 26:CLASS 27:Atom 28:Atom 29:CLASS 30:CLASS 39:CLASS  
40:CLASS 43:CLASS  
44:CLASS 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 58:CLASS  
59:CLASS 60:CLASS  
61:CLASS 62:CLASS 63:CLASS 64:Atom 69:CLASS 71:CLASS 72:CLASS 73:CLASS  
74:CLASS 77:Atom  
79:CLASS

Generic attributes :

40:  
Saturation : Saturated  
47:  
Saturation : Unsaturated  
48:  
Saturation : Unsaturated  
49:  
Saturation : Unsaturated  
50:  
Saturation : Unsaturated  
51:  
Saturation : Unsaturated  
52:  
Saturation : Unsaturated  
64:  
Type of Ring System : Monocyclic  
69:  
Type of chain : Linear  
Saturation : Saturated

L1 STRUCTURE UPLOADED

=> s 11  
SAMPLE SEARCH INITIATED 16:20:52 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 58889 TO ITERATE

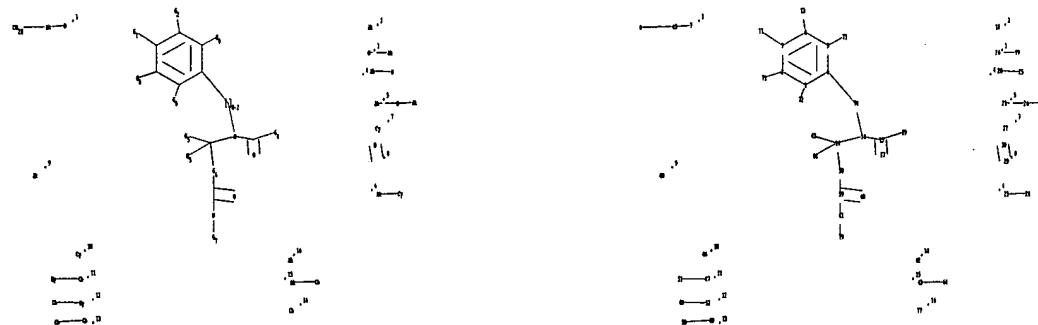
3.4% PROCESSED 2000 ITERATIONS 0 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 1163315 TO 1192245  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=>

Uploading C:\Program Files\Stnexp\Queries\10565557-broad(2).str



chain nodes :

7 8 11 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30  
39 40 43 44 46 47 48 49 50 51 52 58 59 60 61 62 63 64 69 71 72  
73 74 77 79

ring nodes :

1 2 3 4 5 6

chain bonds :

1-72 2-71 3-11 4-13 5-73 6-74 7-69 8-69 14-16 14-15 14-74 15-17 15-39  
16-43 16-44 16-58 19-24 20-25 21-26 22-26 23-28 29-30 47-51 48-52 49-50  
58-59 59-60  
59-61 61-79 63-64

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

1-72 2-71 3-11 4-13 5-73 7-69 8-69 14-16 14-15 14-74 15-17 15-39 16-43  
16-44 16-58 19-24 20-25 21-26 22-26 23-28 29-30 47-51 48-52 58-59 59-60  
59-61 61-79  
63-64

exact bonds :

6-74 49-50

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1:OH,CO2H, [\*1]  
G2:OH,CO2H,H,CH3  
G4:[\*2],[\*3],[\*4],[\*5],[\*6],[\*7],[\*8]  
G5:H, [\*9]  
G6:[\*10],[\*11],[\*12],[\*13]  
G7:[\*14],[\*15],[\*16]  
G8:H,CH3

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 11:CLASS 13:CLASS  
14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS  
22:CLASS 23:CLASS  
24:CLASS 25:CLASS 26:CLASS 27:Atom 28:Atom 29:CLASS 30:CLASS 39:CLASS  
40:CLASS 43:CLASS  
44:CLASS 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 58:CLASS  
59:CLASS 60:CLASS  
61:CLASS 62:CLASS 63:CLASS 64:Atom 69:CLASS 71:CLASS 72:CLASS 73:CLASS  
74:CLASS 77:Atom  
79:CLASS  
Generic attributes :  
40:  
Saturation : Saturated  
47:  
Saturation : Unsaturated  
48:  
Saturation : Unsaturated  
49:  
Saturation : Unsaturated  
50:  
Saturation : Unsaturated  
51:  
Saturation : Unsaturated  
52:  
Saturation : Unsaturated  
64:  
Type of Ring System : Monocyclic  
69:  
Type of chain : Linear  
Saturation : Saturated

L3 STRUCTURE UPLOADED

=> s 13  
SAMPLE SEARCH INITIATED 16:23:12 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 6353 TO ITERATE

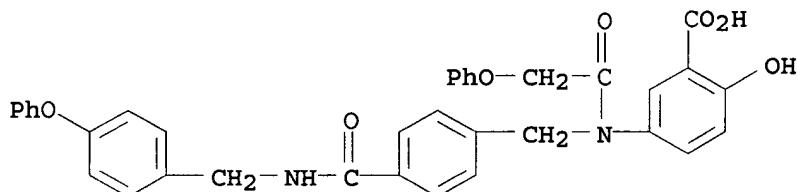
31.5% PROCESSED 2000 ITERATIONS 1 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 122281 TO 131839

L4 1 SEA SSS SAM L3

=&gt; d scan

L4 1 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN  
 IN Benzoic acid, 2-hydroxy-5-[(phenoxyacetyl)[[4-[[[(4-phenoxyphenyl)methyl]amino]carbonyl]phenyl]methyl]amino] - (9CI)  
 MF C36 H30 N2 O7



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> s 13 sss full  
 FULL SEARCH INITIATED 16:23:51 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 129434 TO ITERATE  
 100.0% PROCESSED 129434 ITERATIONS  
 SEARCH TIME: 00.00.03

35 ANSWERS

L5 35 SEA SSS FUL L3

=> sav tem brd565557/a  
 ENTER L#, L# RANGE, ALL, OR (END):15

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	174.80	175.01

FILE 'CAPLUS' ENTERED AT 16:24:21 ON 17 APR 2007  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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 FILE LAST UPDATED: 15 Apr 2007 (20070415/ED)

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L6 6 L5

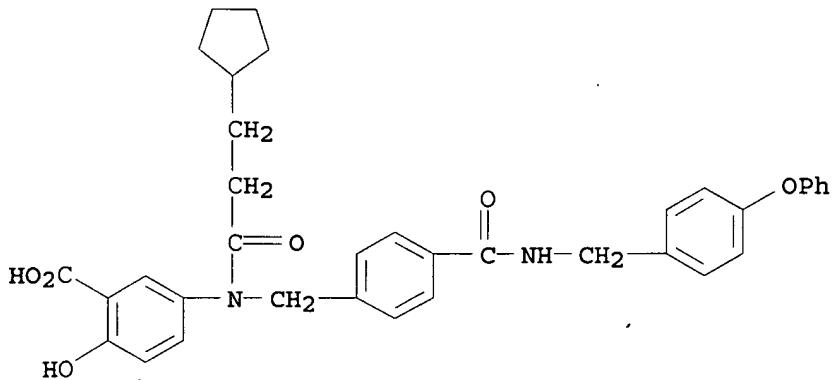
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L6 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN  
AN 2007:87128 CAPLUS <<LOGINID::20070417>>  
DN 146:177185  
TI Glepp-1 inhibitors in the treatment of autoimmune and/or inflammatory  
disorders  
IN Bombrun, Agnes; Hooft van Huijsduijnen, Rob; Jorand-Lebrun, Catherine;  
Vitte, Pierre-Alain; Gerber, Patrick  
PA Applied Research Systems Ars Holding N. V., Neth. Antilles  
SO PCT Int. Appl., 77pp.  
CODEN: PIXXD2

DT Patent  
LA English

FAN.CNT 1

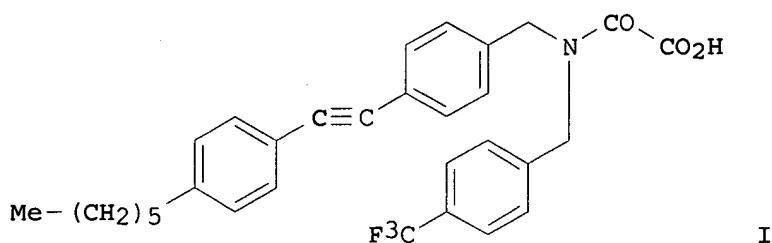
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2007009959	A1	20070125	WO 2006-EP64288	20060714
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
PRAI	EP 2005-106547	A	20050715		
	US 2005-706365P	P	20050808		
OS	MARPAT 146:177185				
AB	The present invention is related to the use of a Glepp-1 inhibitor for the manufacture of a medicament for the treatment of an autoimmune and/or an inflammatory disorder.				
IT	842136-75-8 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (Glepp-1 inhibitors in treatment of autoimmune and/or inflammatory disorders)				
RN	842136-75-8 CAPLUS				
CN	Benzoic acid, 5-[(3-cyclopentyl-1-oxopropyl)[[4-[[[(4- phenoxyphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]-2-hydroxy- (9CI) (CA INDEX NAME)				



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 2005:984019 CAPLUS <<LOGINID::20070417>>  
 DN 143:279395  
 TI Methylene amide derivatives for cardiovascular disorders  
 IN Hooft van Huijsdijnen, Rob; Richard, Vincent  
 PA Applied Research Systems Ars Holding N. V., Neth. Antilles  
 SO PCT Int. Appl., 75 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005082347	A1	20050909	WO 2005-EP50823	20050225
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2005216649	A1	20050909	AU 2005-216649	20050225
	CA 2554919	A1	20050909	CA 2005-2554919	20050225
	EP 1732534	A1	20061220	EP 2005-716814	20050225
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
	CN 1933827	A	20070321	CN 2005-80008722	20050225
	NO 2006004295	A	20060922	NO 2006-4295	20060922
PRAI	EP 2004-100778	A	20040227		
	WO 2005-EP50823	W	20050225		
OS	MARPAT 143:279395				
GI					

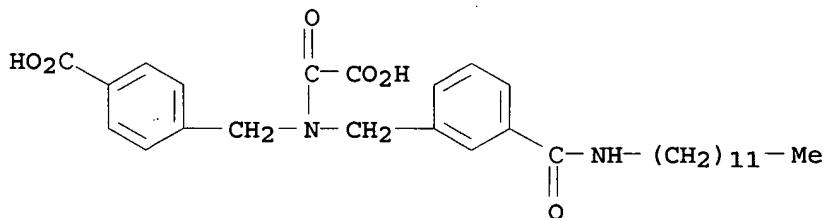


AB The present invention is related to the use of substituted methylene amide derivs. for the treatment and/or prevention of cardiovascular disorders such as coronary obstruction and heart failure and/or prevention of endothelial dysfunction in heart failure. A methylene amide derivative I was able to acutely restore endothelial function in mice with chronic heart failure.

IT 578022-53-4, 4-[[[Carboxycarbonyl] [3-[(dodecylamino) carbonyl]benzyl]amino]methyl]benzoic acid; 578022-58-9, [[3-[(Dodecylamino) carbonyl]benzyl] (4-hydroxybenzyl)amino] (oxo)acetic acid  
 578022-67-0, 4-[[[Carboxycarbonyl] [4-[(dodecylamino) carbonyl]benzyl]amino]methyl]benzoic acid 578022-93-2, [[4-[(Dodecylamino) carbonyl]benzyl] (4-hydroxybenzyl)amino] (oxo)acetic acid  
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (methylene amide derivs. for cardiovascular disorders)

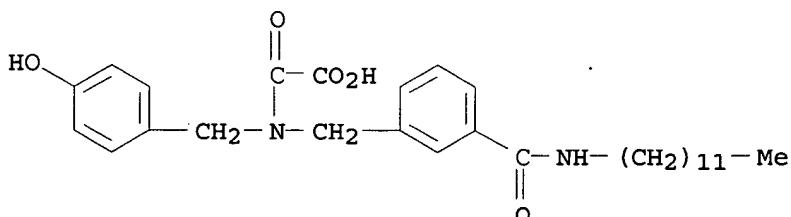
RN 578022-53-4 CAPPLUS

CN Benzoic acid, 4-[[[carboxycarbonyl] [3-[(dodecylamino) carbonyl]phenyl]methyl]amino]methyl] - (9CI) (CA INDEX NAME)



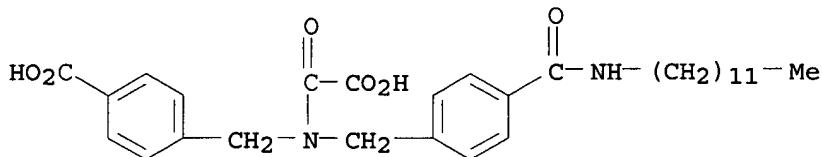
RN 578022-58-9 CAPPLUS

CN Acetic acid, [[3-[(dodecylamino) carbonyl]phenyl]methyl] [(4-hydroxyphenyl)methyl]amino]oxo- (9CI) (CA INDEX NAME)

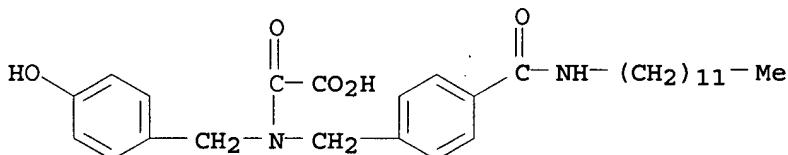


RN 578022-67-0 CAPPLUS

CN Benzoic acid, 4-[[[carboxycarbonyl] [4-[(dodecylamino) carbonyl]phenyl]methyl]amino]methyl] - (9CI) (CA INDEX NAME)



RN 578022-93-2 CAPLUS  
 CN Acetic acid, [[[4-[(dodecylamino)carbonyl]phenyl]methyl] [(4-hydroxyphenyl)methyl]amino]oxo- (9CI) (CA INDEX NAME)



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 2005:120736 .CAPLUS <<LOGINID::20070417>>  
 DN 142:219051  
 TI Preparation of aryl dicarboxamides as protein-tyrosine phosphatase inhibitors  
 IN Thomas, Russel J.; Swinnen, Dominique; Pons, Jean-Francois; Bombrun, Agnes  
 PA Applied Research Systems Ars Holding N.V., Neth.  
 SO PCT Int. Appl., 103 pp.  
 CODEN: PIXXD2

DT Patent  
 LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005011685	A1	20050210	WO 2004-EP51558	20040720
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004260831	A1	20050210	AU 2004-260831	20040720
	CA 2529662	A1	20050210	CA 2004-2529662	20040720
	EP 1656139	A1	20060517	EP 2004-742005	20040720
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
	JP 2006528157	T	20061214	JP 2006-520836	20040720
	US 2006189583	A1	20060824	US 2006-565557	20060123
	NO 2006000815	A	20060220	NO 2006-815	20060220
PRAI	EP 2003-102236	A	20030721		
	US 2003-517824P	P	20031106		
	WO 2004-EP51558	W	20040720		
OS	CASREACT 142:219051; MARPAT 142:219051				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

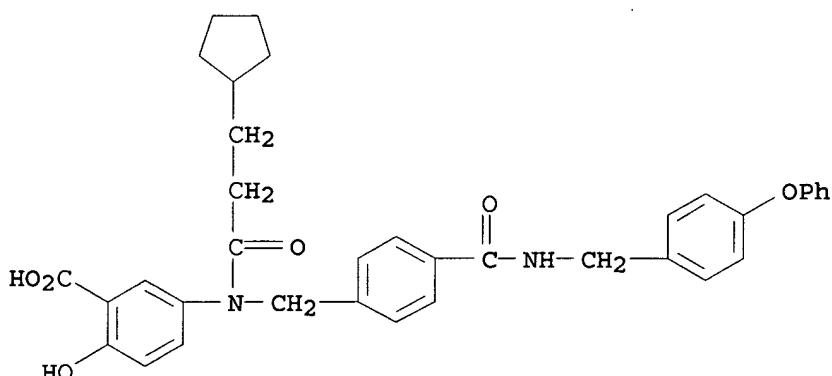
AB Title compds. I [A = CONHR<sub>6</sub> wherein R<sub>6</sub> = alkyl, alkenyl, alkynyl, cycloalkyl, etc.; X = aryl, heteroaryl, arylheteroaryl, arylaryl, etc.; n = 0 or 1; R<sub>1</sub> and R<sub>2</sub> independently = H or alkyl; R<sub>3</sub> = alkyl, alkenyl, alkynyl, alkoxy, etc.; R<sub>4</sub> and R<sub>5</sub> independently = H, OH, alkyl, carboxy, alkoxy, etc.], and their pharmaceutically acceptable salts, are prepared and disclosed as protein-tyrosine phosphatase inhibitors. Thus, e.g., II was prepared via reductive amination of 6-amino-2,2-dimethyl-4H-1,3-benzodioxin-4-one (preparation given) with 4-formylbenzoate and subsequent amidation with 3-cyclopentylpropanoyl chloride, debenzylation, amidation with 4-phenoxybenzylamine and deprotection. I were evaluated for inhibition of PTP, and in particular PTP1B; e.g., II possessed an IC<sub>50</sub> value of 1.0  $\mu$ M in assays against PTP1B. As PTP inhibitors, I should be useful for the treatment and/or prevention of obesity and/or metabolic disorders mediated by insulin resistance or hyperglycemia, comprising diabetes type I and/or II, inadequate glucose tolerance, insulin resistance, hyperlipidemia, hypertriglyceridemia, hypercholesterolemia, polycystic ovary syndrome (PCOS).

IT 842136-75-8P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(drug candidate; preparation of aryl dicarboxamides as protein-tyrosine phosphatase (PTP) inhibitors)

RN 842136-75-8 CAPLUS

CN Benzoic acid, 5-[(3-cyclopentyl-1-oxopropyl)[[4-[(4-phenoxyphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]-2-hydroxy- (9CI)  
(CA INDEX NAME)



IT 842136-78-1P 842136-83-8P 842136-84-9P  
842136-85-0P 842136-86-1P 842136-87-2P  
842136-88-3P 842136-89-4P 842136-90-7P  
842136-91-8P 842136-93-0P 842136-95-2P  
842136-97-4P 842136-99-6P 842137-01-3P  
842137-03-5P 842137-04-6P 842137-05-7P  
842137-07-9P 842137-09-1P 842137-11-5P  
842137-13-7P 842137-14-8P 842137-15-9P  
842137-17-1P 842137-18-2P 842137-19-3P  
842137-20-6P 842137-21-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)

(drug candidate; preparation of aryl dicarboxamides as protein-tyrosine phosphatase (PTP) inhibitors)

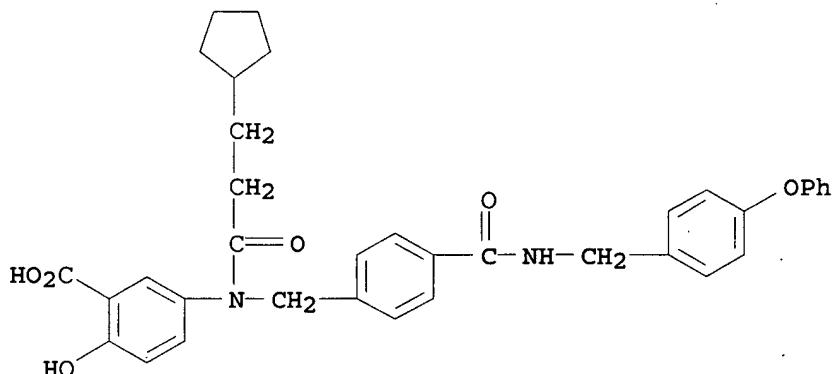
RN 842136-78-1 CAPLUS

CN D-Glucitol, 1-deoxy-1-(methylamino)-, 5-[(3-cyclopentyl-1-oxopropyl)[[4-[[[(4-phenoxyphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]-2-hydroxybenzoate (salt) (9CI) (CA INDEX NAME)

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CRN 842136-75-8

CMF C36 H36 N2 O6

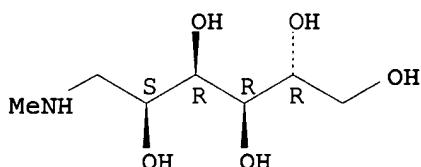


CM 2

CRN 6284-40-8

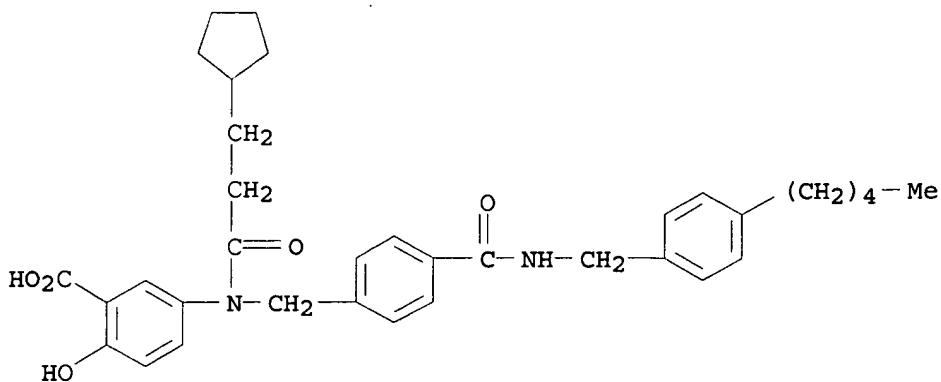
CMF C7 H17 N O5

Absolute stereochemistry.

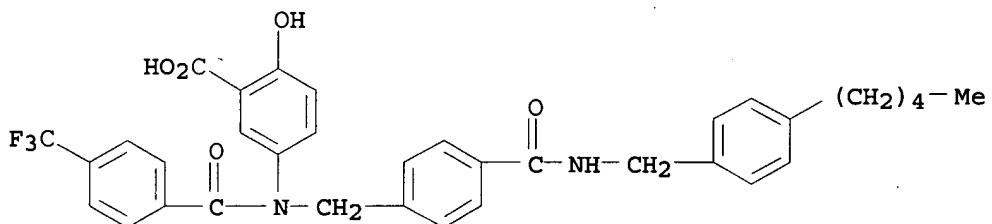


RN 842136-83-8 CAPLUS

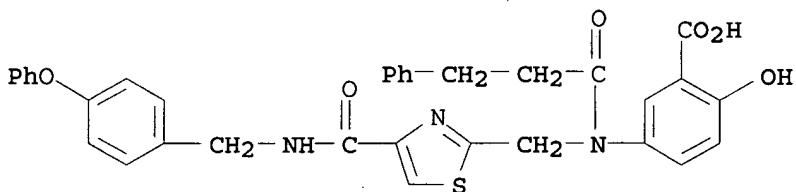
CN Benzoic acid, 5-[(3-cyclopentyl-1-oxopropyl)[[4-[[[(4-pentylphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]-2-hydroxy- (9CI) (CA INDEX NAME)



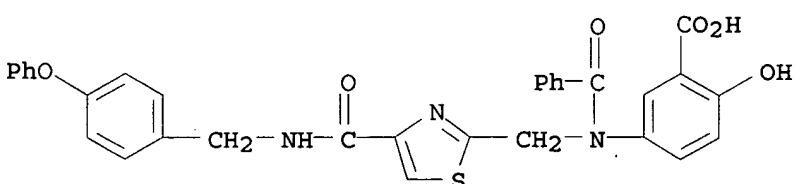
RN 842136-84-9 CAPLUS  
 CN Benzoic acid, 2-hydroxy-5-[[[4-[[[4-pentylphenyl]methyl]amino]carbonyl]phenyl]methyl] [4-(trifluoromethyl)benzoyl]amino]- (9CI) (CA INDEX NAME)



RN 842136-85-0 CAPLUS  
 CN Benzoic acid, 2-hydroxy-5-[(1-oxo-3-phenylpropyl)[[4-[[[4-phenoxyphenyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]amino]- (9CI) (CA INDEX NAME)

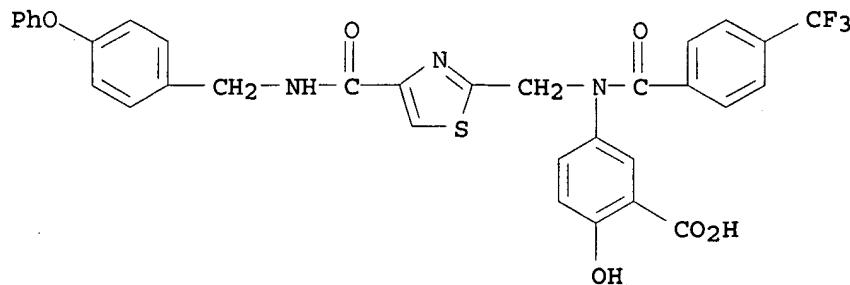


RN 842136-86-1 CAPLUS  
 CN Benzoic acid, 5-[benzoyl[[4-[[[4-phenoxyphenyl]methyl]amino]carbonyl]-2-thiazolyl]methyl]amino]-2-hydroxy- (9CI) (CA INDEX NAME)



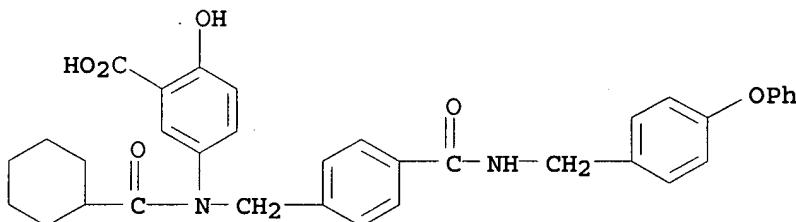
RN 842136-87-2 CAPLUS

CN Benzoic acid, 2-hydroxy-5-[[[4-[[[(4-phenoxyphenyl)methyl]amino]carbonyl]-2-thiazolyl]methyl][4-(trifluoromethyl)benzoyl]amino]- (9CI) (CA INDEX NAME)



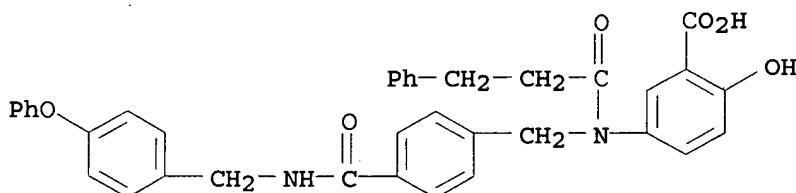
RN 842136-88-3 CAPLUS

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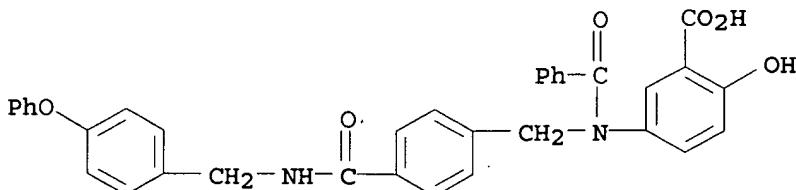
RN 842136-89-4 CAPLUS

CN Benzoic acid, 2-hydroxy-5-[(1-oxo-3-phenylpropyl)[[4-[[[(4-phenoxyphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

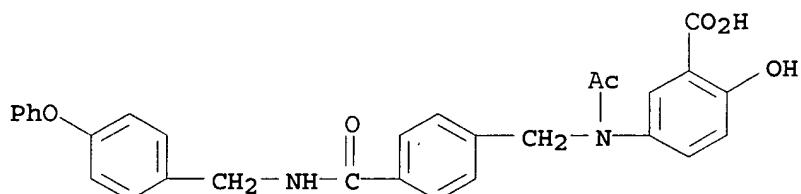


RN 842136-90-7 CAPLUS

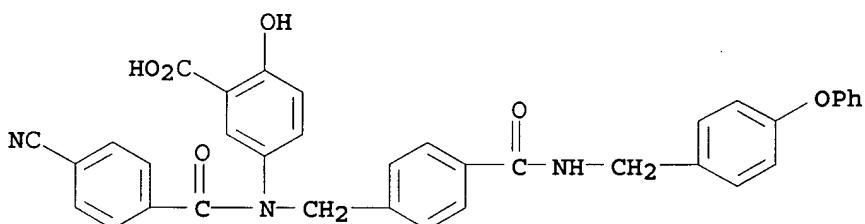
CN Benzoic acid, 5-[[benzoyl[[4-[[[(4-phenoxyphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]-2-hydroxy- (9CI) (CA INDEX NAME)



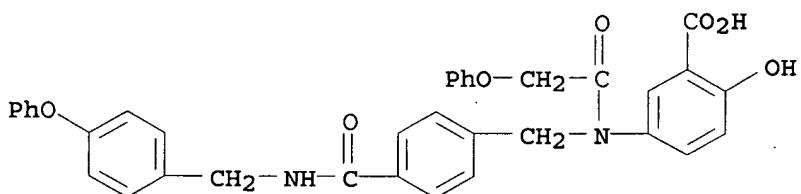
RN 842136-91-8 CAPLUS  
CN Benzoic acid, 5-[acetyl[[4-[[[(4-phenoxyphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]-2-hydroxy- (9CI) (CA INDEX NAME)



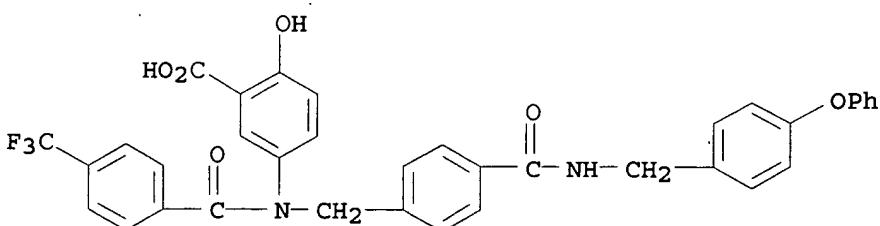
RN 842136-93-0 CAPLUS  
CN Benzoic acid, 5-[(4-cyanobenzoyl)[[4-[[[(4-phenoxyphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]-2-hydroxy- (9CI) (CA INDEX NAME)



RN 842136-95-2 CAPLUS  
CN Benzoic acid, 2-hydroxy-5-[(phenoxyacetyl)[[4-[[[(4-phenoxyphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

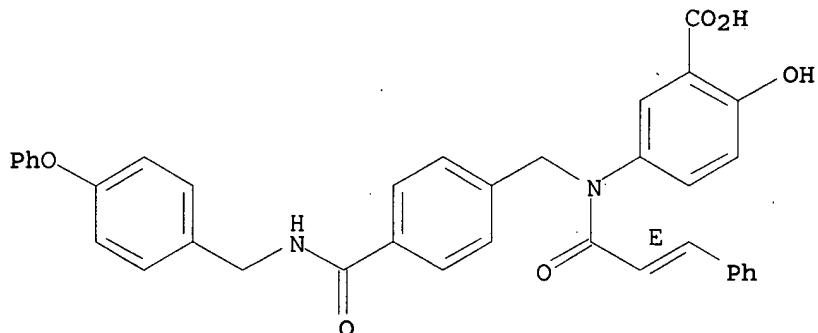


RN 842136-97-4 CAPLUS  
CN Benzoic acid, 2-hydroxy-5-[[[4-[[[(4-phenoxyphenyl)methyl]amino]carbonyl]phenyl]methyl][4-(trifluoromethyl)benzoyl]amino]- (9CI) (CA INDEX NAME)

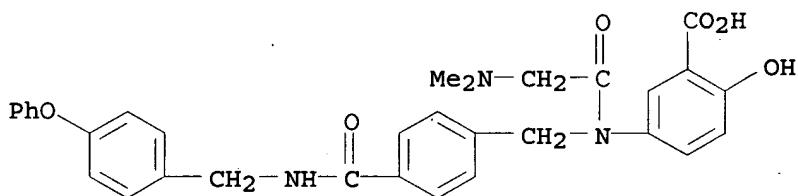


RN 842136-99-6 CAPLUS  
CN Benzoic acid, 2-hydroxy-5-[(2E)-1-oxo-3-phenyl-2-propenyl] [[4-[(4-phenoxyphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

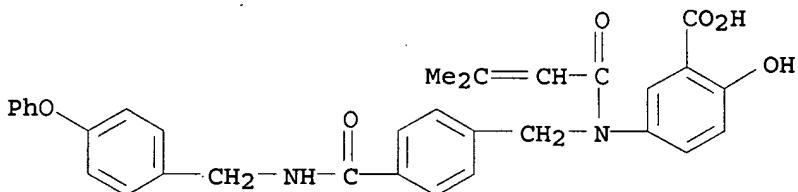
Double bond geometry as shown.



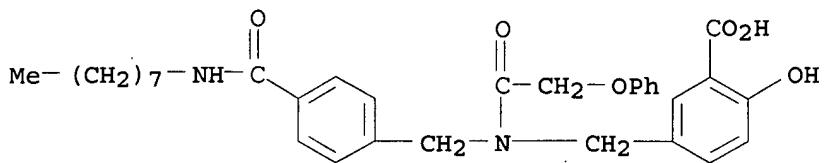
RN 842137-01-3 CAPLUS  
CN Benzoic acid, 5-[(dimethylamino)acetyl][4-[(4-phenoxyphenyl)methyl]amino]carbonylphenylmethyl]amino]-2-hydroxy- (9CI)  
(CA INDEX NAME)



RN 842137-03-5 CAPLUS  
CN Benzoic acid, 2-hydroxy-5-[(3-methyl-1-oxo-2-butenyl){[4-[([(4-phenoxyphenyl)methyl]amino]carbonyl]phenyl}methyl]amino]- (9CI) (CA INDEX NAME)

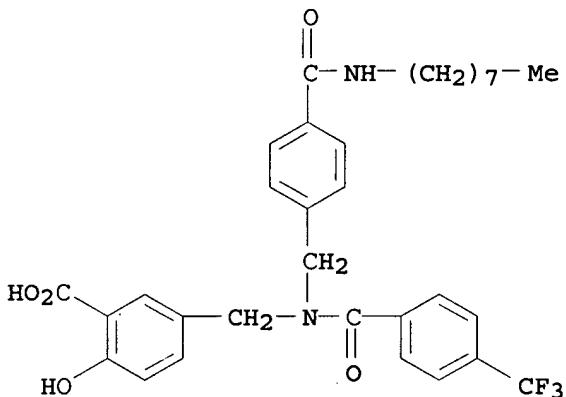


RN 842137-04-6 CAPLUS  
CN Benzoic acid, 2-hydroxy-5-[[[4-[(octylamino)carbonyl]phenyl]methyl](phenoxyacetyl)amino]methyl]- (9CI) (CA INDEX NAME)



RN 842137-05-7 CAPLUS

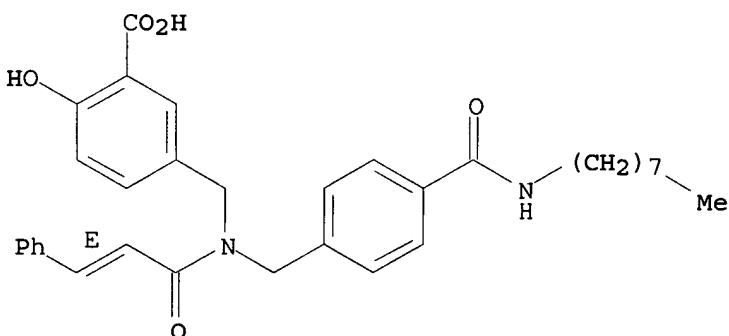
CN Benzoic acid, 2-hydroxy-5-[[[4-[(octylamino)carbonyl]phenyl]methyl][4-(trifluoromethyl)benzoyl]amino]methyl]- (9CI) (CA INDEX NAME)



RN 842137-07-9 CAPLUS

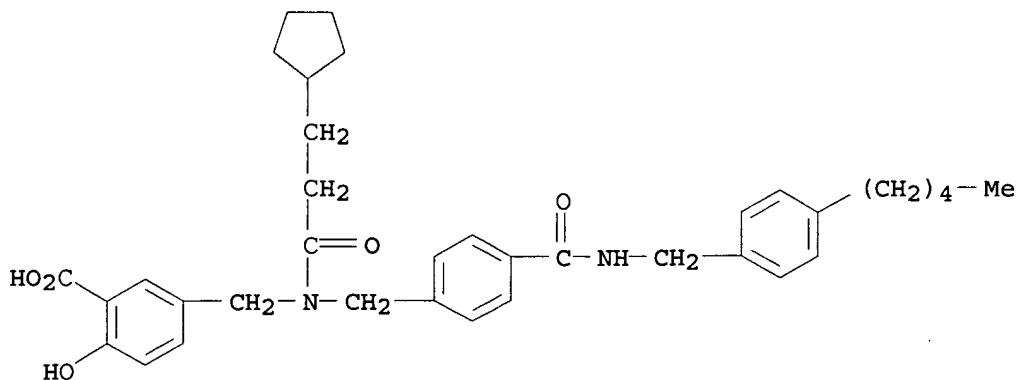
CN Benzoic acid, 2-hydroxy-5-[[[4-[(octylamino)carbonyl]phenyl]methyl][(2E)-1-oxo-3-phenyl-2-propenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



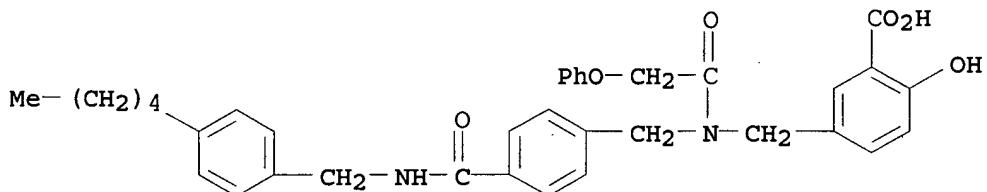
RN 842137-09-1 CAPLUS

CN Benzoic acid, 5-[[[(3-cyclopentyl-1-oxopropyl)[[4-[[[(4-pentylphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]methyl]-2-hydroxy- (9CI) (CA INDEX NAME)



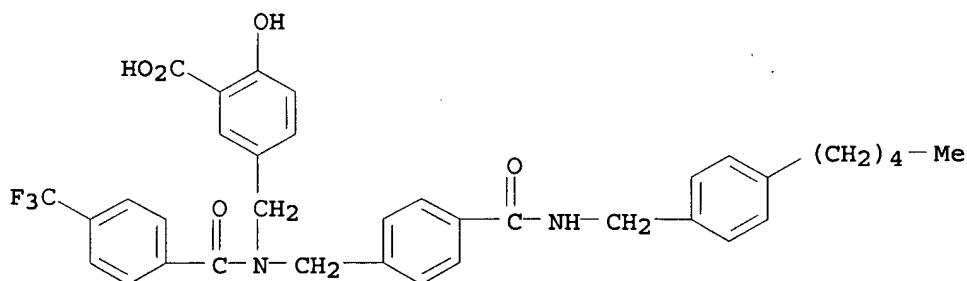
RN 842137-11-5 CAPLUS

CN Benzoic acid, 2-hydroxy-5-[[[4-[[[4-pentylphenyl)methyl]amino]carbonyl]phenyl]methyl](phenoxyacetyl)amino]methyl] - (9CI) (CA INDEX NAME)



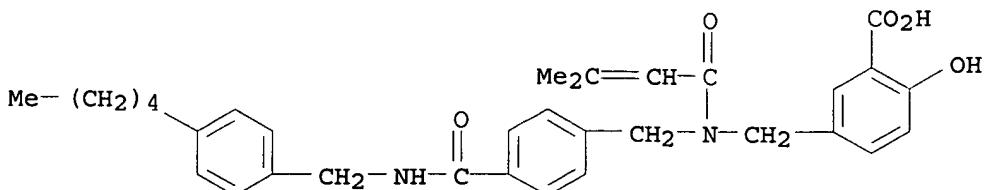
RN 842137-13-7 CAPLUS

CN Benzoic acid, 2-hydroxy-5-[[[4-[[[4-pentylphenyl)methyl]amino]carbonyl]phenyl]methyl][4-(trifluoromethyl)benzoyl]amino]methyl]- (9CI) (CA INDEX NAME)

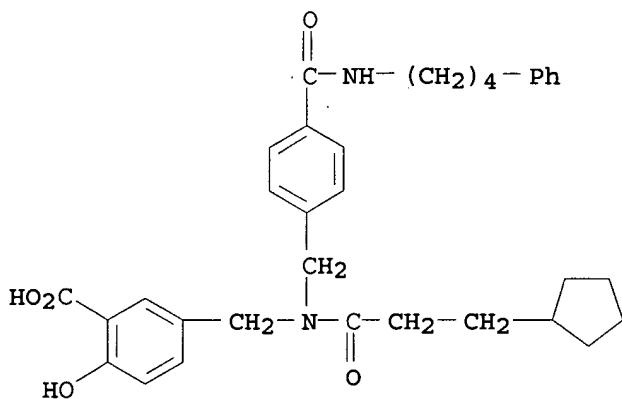


RN 842137-14-8 CAPLUS

CN Benzoic acid, 2-hydroxy-5-[(3-methyl-1-oxo-2-butenyl)[[4-[([(4-pentylphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]methyl]- (9CI) (CA INDEX NAME)

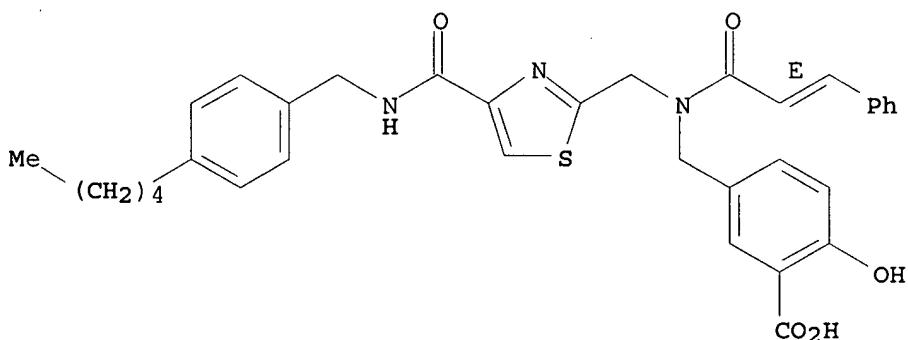


RN 842137-15-9 CAPLUS  
 CN Benzoic acid, 5-[[[(3-cyclopentyl-1-oxopropyl) [[4-[[[(4-phenylbutyl)amino]carbonyl]phenyl]methyl]amino]methyl]-2-hydroxy- (9CI)  
 (CA INDEX NAME)

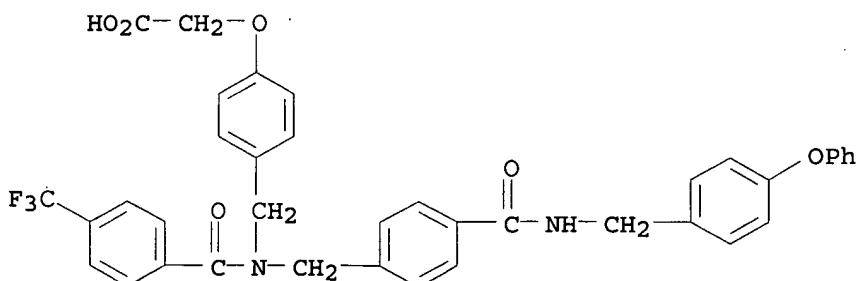


RN 842137-17-1 CAPLUS  
 CN Benzoic acid, 2-hydroxy-5-[[[(2E)-1-oxo-3-phenyl-2-propenyl] [[4-[[[(4-pentylphenyl)methyl]amino]carbonyl]-2-thiazolyl]methyl]amino]methyl]- (9CI) (CA INDEX NAME)

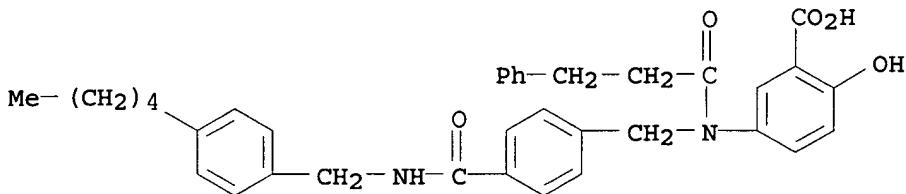
Double bond geometry as shown.



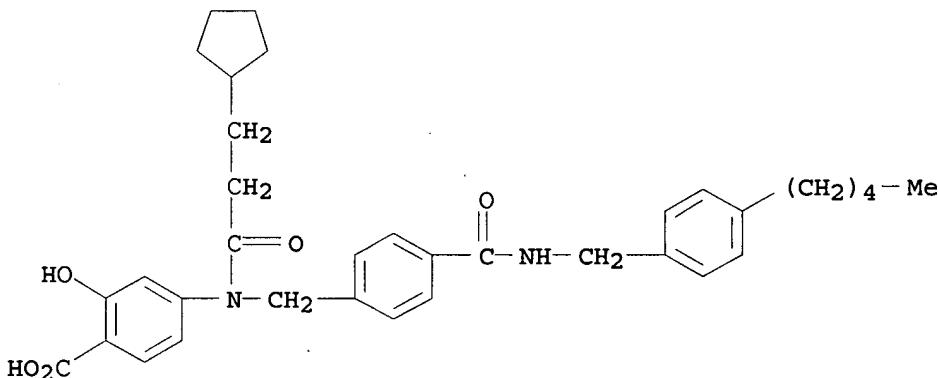
RN 842137-18-2 CAPLUS  
 CN Acetic acid, [4-[[[[[4-[[[(4-phenoxyphenyl)methyl]amino]carbonyl]phenyl]methyl] [4-(trifluoromethyl)benzoyl]amino]methyl]phenoxy]- (9CI) (CA INDEX NAME)



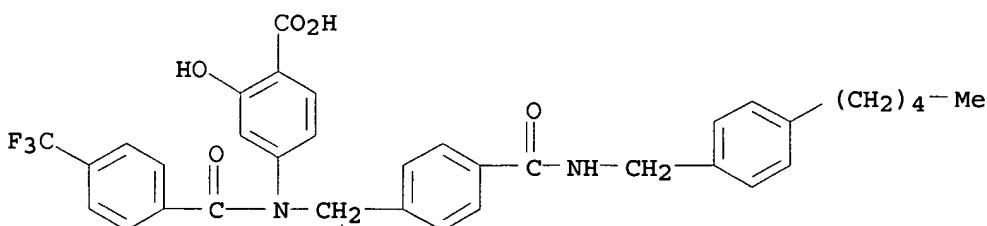
RN 842137-19-3 CAPLUS  
 CN Benzoic acid, 2-hydroxy-5-[(1-oxo-3-phenylpropyl)[[4-[[[(4-pentylphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]- (9CI) (CA INDEX NAME)



RN 842137-20-6 CAPLUS  
 CN Benzoic acid, 4-[(3-cyclopentyl-1-oxopropyl)[[4-[[[(4-pentylphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]-2-hydroxy- (9CI) (CA INDEX NAME)



RN 842137-21-7 CAPLUS  
 CN Benzoic acid, 2-hydroxy-4-[[[4-[[[(4-pentylphenyl)methyl]amino]carbonyl]phenyl]methyl][4-(trifluoromethyl)benzoyl]amino]- (9CI) (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 2003:610410 CAPLUS <<LOGINID::20070417>>  
 DN 139:179889  
 TI Methylene amides, particularly [(aryl methyl)amino] (oxo) acetic acids, useful as modulators, and especially inhibitors, of protein tyrosine

phosphatases (PTPs), and their preparation, uses, e.g., as antidiabetics, and pharmaceutical compositions.

IN Swinnen, Dominique; Bombrun, Agnes; Gonzalez, Jerome; Gerber, Patrick; Pittet, Pierre-Andre

PA Applied Research Systems ARS Holding N.V., Neth. Antilles

SO PCT Int. Appl., 346 pp.

CODEN: PIXXD2

DT Patent

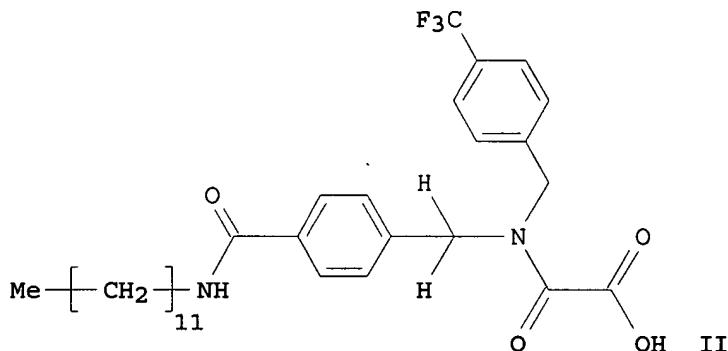
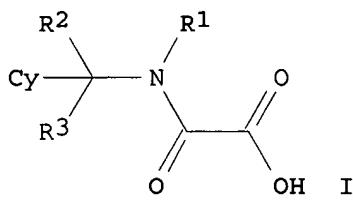
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003064376	A1	20030807	WO 2003-EP808	20030127
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2472021	A1	20030807	CA 2003-2472021	20030127
	EP 1470102	A1	20041027	EP 2003-734697	20030127
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	BR 2003007394	A	20041109	BR 2003-7394	20030127
	JP 2005516061	T	20050602	JP 2003-564000	20030127
	US 2005124656	A1	20050609	US 2003-501344	20030127
	CN 1633410	A	20050629	CN 2003-807036	20030127
	ZA 2004005179	A	20050629	ZA 2004-5179	20040629
	IN 2004DN01884	A	20070406	IN 2004-DN1884	20040701
	NO 2004003520	A	20041005	NO 2004-3520	20040824
PRAI	EP 2002-100078	A	20020129		
	EP 2002-100410	A	20020425		
	WO 2003-EP808	W	20030127		

OS MARPAT 139:179889

GI



AB Title compds. I [wherein R1 = alkyl, alkenyl, alkynyl, aryl, heteroaryl, (3-8-membered)-cycloalkyl, heterocycloalkyl, (alkyl)aryl, (alkyl)heteroaryl, (alkenyl)aryl, heteroaryl, (alkynyl)aryl, heteroaryl; R2, R3 = independently H or alkyl; Cy = aryl, heteroaryl, cycloalkyl, heterocyclyl; with the proviso that four compds. are excluded; their geometrical isomers, optically active forms as enantiomers, diastereomers and racemates, and pharmaceutically acceptable salts and active derivs.] were prepared as inhibitors of protein tyrosine phosphatases (PTPs), in particular PTP1B. Examples include over 400 invention compds., five pharmaceutical formulations, and two biol. assays. For example, II was prepared in 4 steps by amidation of 4-formylbenzoic acid with dodecylamine in THF in the presence of 4-methylmorpholine and iso-Bu chloroformate for 3 h at room temperature, reductive amination with 4-trifluoromethylbenzylamine in DCE in the presence of NaBH(OAc)3, TEA-acylation with chlorooxoacetic acid Et ester in THF, and base-catalyzed hydrolysis of the ester. II exhibited an IC50 value of 2.224  $\mu\text{M}$  for inhibition of PTP1B, 1.40  $\mu\text{M}$  for GLEPP-1, 2.40  $\mu\text{M}$  for SHP-1, and 2.70  $\mu\text{M}$  for SHP-2 in an in vitro assay. In an in vivo postprandial glycemia model in db/db mice, II, at 20-200 mg/kg orally, decreased blood glucose level by 17% at 20 mg/kg, by 42% at 100 mg/kg, and by 48% at 200 mg/kg, with decreases in serum insulin levels of -2%, 66%, and 89%, resp. Thus, I and their formulations are useful for the treatment and/or prevention of metabolic disorders mediated by insulin resistance or hyperglycemia, comprising diabetes type I and/or II, inadequate glucose tolerance, insulin resistance, hyperlipidemia, hypertriglyceridemia, hypercholesterolemia, obesity, polycystic ovary syndrome (PCOS).

IT 578022-53-4P, 4-[[[Carboxycarbonyl] [3-[(dodecylamino) carbonyl] benzyl] amino] methyl] benzoic acid  
 578022-58-9P, [[3-[(Dodecylamino) carbonyl] benzyl] (4-hydroxybenzyl) amino] (oxo) acetic acid 578022-67-0P, 4-[[[Carboxycarbonyl] [4-[(dodecylamino) carbonyl] benzyl] amino] methyl] benzoic acid 578022-93-2P, [[4-[(Dodecylamino) carbonyl] benzyl] (4-hydroxybenzyl) amino] (oxo) acetic acid

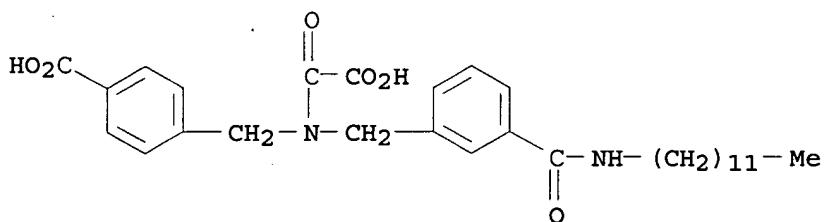
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of [(arylmethyl)amino] (oxo) acetic acids as PTP

inhibitors for antidiabetics)

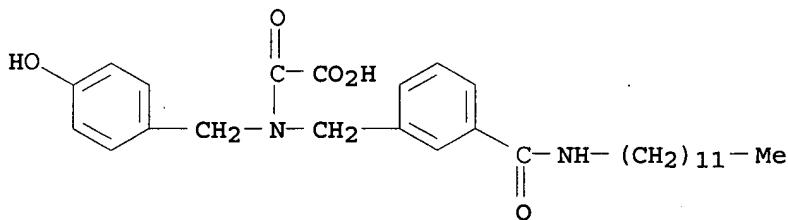
RN 578022-53-4 CAPLUS

CN Benzoic acid, 4-[[[(carboxycarbonyl) [[3-[(dodecylamino) carbonyl]phenyl]methoxy]amino]methyl]- (9CI) (CA INDEX NAME)



RN 578022-58-9 CAPLUS

CN Acetic acid, [[[3-[(dodecylamino) carbonyl]phenyl]methyl] [(4-hydroxyphenyl)methyl]amino]oxo- (9CI) (CA INDEX NAME)

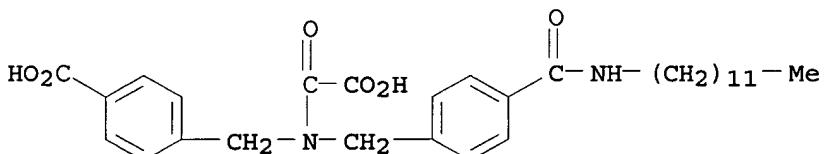


not 103 blc  
112  $\Rightarrow$  unfldictable  
activity 50

not motivated to  
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expectation of  
success)

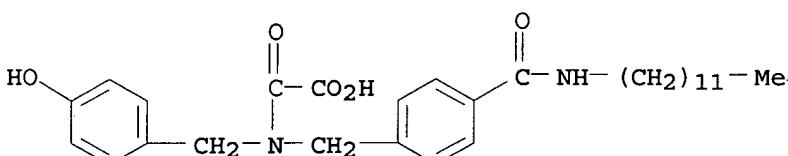
RN 578022-67-0 CAPLUS

CN Benzoic acid, 4-[[[(carboxycarbonyl) [[4-[(dodecylamino) carbonyl]phenyl]methoxy]amino]methyl]- (9CI) (CA INDEX NAME)



RN 578022-93-2 CAPLUS

CN Acetic acid, [[[4-[(dodecylamino) carbonyl]phenyl]methyl] [(4-hydroxyphenyl)methyl]amino]oxo- (9CI) (CA INDEX NAME)

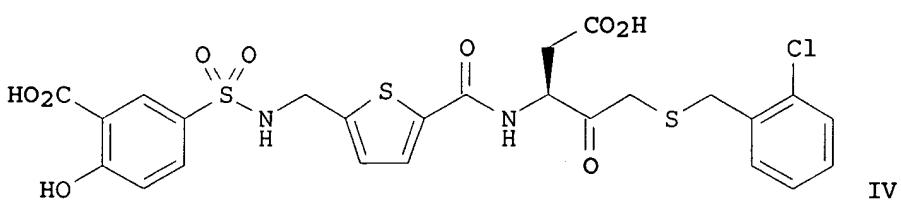
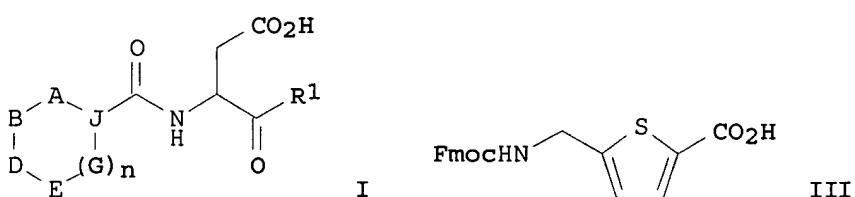


RE.CNT 7

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN  
 AN 2003:242322 CAPLUS <>LOGINID::20070417>>  
 DN 138:271968  
 TI Preparation of (heterocyclylcarbonyl) aspartic acid derivatives as caspase inhibitors  
 IN Choong, Ingrid; Burdett, Matthew; Delano, Warren; Erlanson, Daniel A.;  
 Lee, Dennis; Lew, Willard  
 PA Sunesis Pharmaceuticals, Inc., USA  
 SO PCT Int. Appl., 179 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003024955	A2	20030327	WO 2002-US29536	20020917
	WO 2003024955	A3	20030814		
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 2003114447	A1	20030619	US 2002-245912	20020917
	US 6878743	B2	20050412		
OS	US 2001-323270P	P	20010918		
	US 2002-371762P	P	20020411		
GI	MARPAT 138:271968				



AB The present invention provides aspartic acid derivs. I [R1 = H, aliphatic, heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl, heteroalkylaryl, heteroalkylheteroaryl; n = 0, 1; A, B, D, E, G, = independently CR, CR2, CO, S, NR, NR2, O; J = CR; each R = independently H, halo, OR2, NR22, SR2, CN, CO2R2, COR2, CONR22, SOR2, SO2R2, SO2NR22, NR2SO2R2, O2CNR22, NR2CONR22, NR2CSNR22, NR2SO2NR22, (un)substituted

aliphatic, heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl, heteroalkylaryl, heteroalkylheteroaryl; R2 = independently H, halo, OR3, NR32, SR3, CN, CO2R3, COR3, CONR32, SOR3, SO2R3, SO2NR32, NR3SO2R3, O2CNR32, NR3CONR32, NR3CSNR32, NR3SO2NR32, (un)substituted aliphatic, heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl, heteroalkylaryl, heteroalkylheteroaryl; R3 = H, aliphatic, heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl, heteroalkylaryl, heteroalkylheteroaryl; with provisos] and pharmaceutically acceptable derivs., and pharmaceutical compns. thereof, and methods for the use thereof as caspase inhibitors and for the treatment of disorders caused by excessive apoptotic activity (no data). Thus, Fmoc-Asp(OtBu)-CH2Br (Fmoc = 9-fluorenylmethoxycarbonyl) was coupled with 2-ClC6H4CH2SH to give sulfide Fmoc-Asp(OtBu)CH2SCH2C6H4Cl-2 (II). II was attached to a semicarbazide-derivatized Wang resin, deprotected with piperidine in DMF, coupled with Fmoc-protected aminomethylthiophenecarboxylic acid III, deprotected, and coupled with 5-chlorosulfonyl-2-hydroxybenzoic acid, and cleaved from the resin with CF3CO2H to give inhibitor IV.

IT

476362-87-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (heterocyclcarbonyl)aspartic acid derivs. as caspase inhibitors)

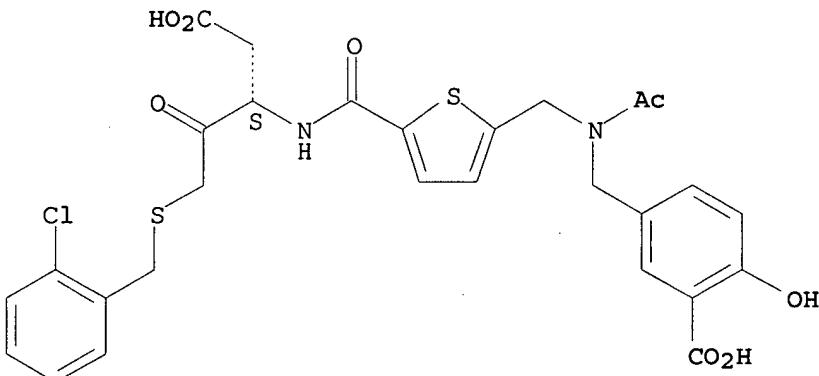
RN

476362-87-5 CAPLUS

CN

Benzoic acid, 5-[[acetyl[[5-[[[(1S)-1-(carboxymethyl)-3-[[[(2-chlorophenyl)methyl]thio]-2-oxopropyl]amino]carbonyl]-2-thienyl]methyl]amino]methyl]-2-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:782787 CAPLUS <<LOGINID::20070417>>

DN 138:98

TI Identification of potent and selective small-molecule inhibitors of caspase-3 through the use of extended tethering and structure-based drug design

AU Choong, Ingrid C.; Lew, Willard; Lee, Dennis; Pham, Phuongly; Burdett, Matthew T.; Lam, Joni W.; Wiesmann, Christian; Luong, Tinh N.; Fahr, Bruce; DeLano, Warren L.; McDowell, Robert S.; Allen, Darin A.; Erlanson, Daniel A.; Gordon, Eric M.; O'Brien, Tom

CS Sunesis Pharmaceuticals Inc., South San Francisco, CA, 94080, USA

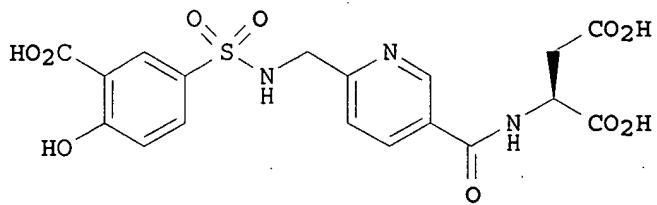
SO Journal of Medicinal Chemistry (2002), 45(23), 5005-5022

CODEN: JMCMAR; ISSN: 0022-2623

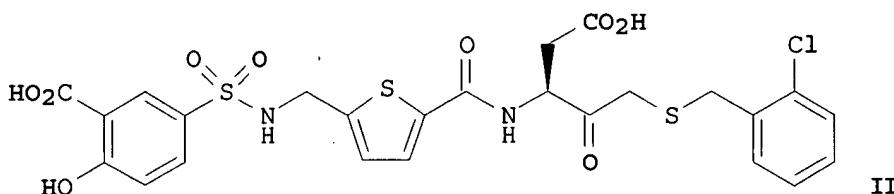
PB American Chemical Society

DT Journal

LA English



I



II

AB The design, synthesis, and in vitro activities of a series of potent and selective small-mol. inhibitors of caspase-3 are described. From extended tethering, a salicylic acid fragment was identified as having binding affinity for the S4 pocket of caspase-3. X-ray crystallog. and mol. modeling of the initial tethering hit resulted in the synthesis of (I), which reversibly inhibited caspase-3 with a  $K_i = 40$  nM. Further optimization led to the identification of a series of potent and selective inhibitors with  $K_i$  values in the 20-50 nM range. One of the most potent compds. in this series, (II), inhibited caspase-3 with a  $K_i = 20$  nM and selectivity of 8-500-fold for caspase-3 vs a panel of seven caspases (1, 2, and 4-8). A high-resolution X-ray cocrystal structure of I and II supports the predicted binding modes of our compds. with caspase-3.

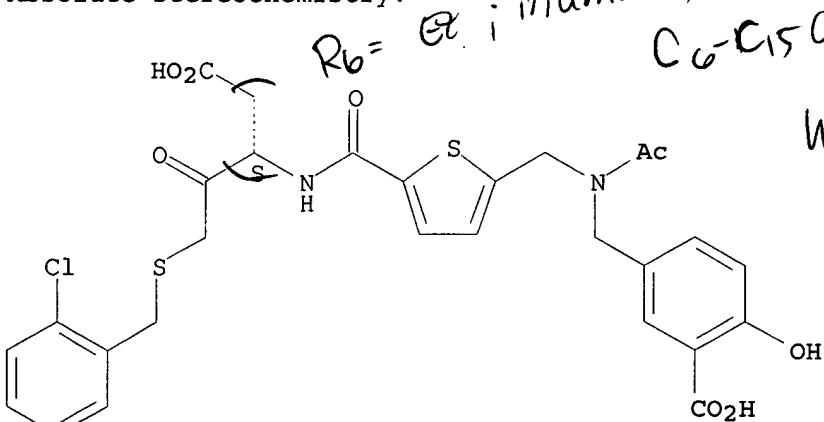
IT 476362-87-5P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (identification of potent and selective small-mol. inhibitors of caspase-3 through the use of extended tethering and structure-based drug design)

RN 476362-87-5 CAPLUS

CN Benzoic acid, 5-[[acetyl[[5-[[[(1S)-1-(carboxymethyl)-3-[[[(2-chlorophenyl)methyl]thio]-2-oxopropyl]amino]carbonyl]-2-thienyl]methyl]amino]methyl]-2-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



Affinity

RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 16:20:09 ON 17 APR 2007)

FILE 'REGISTRY' ENTERED AT 16:20:17 ON 17 APR 2007

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L3 STRUCTURE uploaded  
L4 1 S L3  
L5 35 S L3 SSS FULL  
SAV TEM BRD565557/A L5

FILE 'CAPLUS' ENTERED AT 16:24:21 ON 17 APR 2007

L6 6 S L5

=> sav tem ans565557/a 16

=> log hold

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FULL ESTIMATED COST	32.56	207.57
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.68	-4.68

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 16:25:15 ON 17 APR 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptasj11626

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'CAPLUS' AT 16:48:30 ON 17 APR 2007  
FILE 'CAPLUS' ENTERED AT 16:48:30 ON 17 APR 2007  
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

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FULL ESTIMATED COST	32.56	207.57
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CA SUBSCRIBER PRICE	-4.68	-4.68

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CA SUBSCRIBER PRICE

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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provided by InfoChem.

STRUCTURE FILE UPDATES: 16 APR 2007 HIGHEST RN 930395-50-9  
DICTIONARY FILE UPDATES: 16 APR 2007 HIGHEST RN 930395-50-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

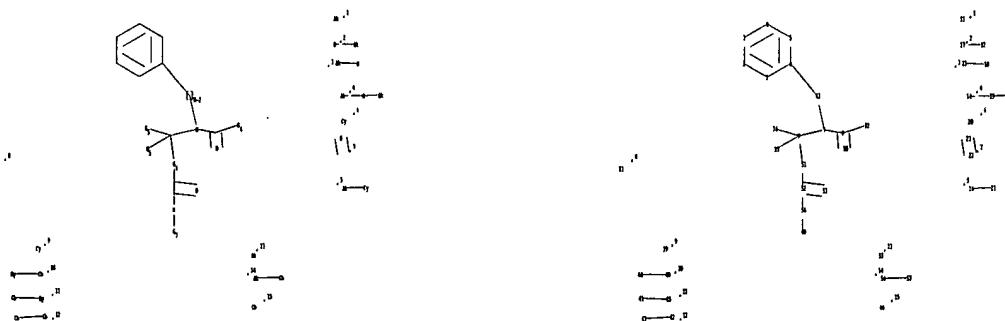
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

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chain nodes :  
7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 32 33 36 37  
39 40 41 42 43 44 45 51 52 53 54 55 56 57 63 66 68  
ring nodes :  
1 2 3 4 5 6  
chain bonds :  
6-63 7-9 7-8 7-63 8-10 8-32 9-36 9-37 9-51 12-17 13-18 14-19 15-19  
16-21  
22-23 40-44 41-45 42-43 51-52 52-53 52-54 54-68 56-57  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
7-9 7-8 7-63 8-10 8-32 9-36 9-37 9-51 12-17 13-18 14-19 15-19 16-21  
22-23 40-44 41-45 51-52 52-53 52-54 54-68 56-57  
exact bonds :  
6-63 42-43  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

G4:[\*1],[\*2],[\*3],[\*4],[\*5],[\*6],[\*7]

G5:H,[\*8]

G6:[\*9],[\*10],[\*11],[\*12]

G7:[\*13],[\*14],[\*15]

G8:H,CH3

G9:O

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:Atom  
21:Atom 22:CLASS 23:CLASS 32:CLASS 33:CLASS 36:CLASS 37:CLASS 39:Atom  
40:Atom 41:Atom  
42:Atom 43:Atom 44:Atom 45:Atom 51:CLASS 52:CLASS 53:CLASS 54:CLASS  
55:CLASS 56:CLASS 57:Atom  
63:CLASS 66:Atom 68:CLASS  
Generic attributes :  
33:  
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40:  
Saturation : Unsaturated  
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42:  
Saturation : Unsaturated  
43:  
Saturation : Unsaturated  
44:  
Saturation : Unsaturated  
45:  
Saturation : Unsaturated  
57:  
Type of Ring System : Monocyclic

L7 STRUCTURE UPLOADED

=> s 17  
SAMPLE SEARCH INITIATED 16:48:55 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 15766 TO ITERATE

12.7% PROCESSED 2000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 307800 TO 322840  
PROJECTED ANSWERS: 913 TO 1923

L8 9 SEA SSS SAM L7

=> s 17 sss full  
FULL SEARCH INITIATED 16:49:06 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 321203 TO ITERATE

100.0% PROCESSED 321203 ITERATIONS  
SEARCH TIME: 00.00.08

L9 855 SEA SSS FUL L7

=> sav tem brI565557/a  
ENTER L#, L# RANGE, ALL, OR (END):19

=> fil stng  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 172.55 380.12  
  
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL  
ENTRY SESSION  
CA SUBSCRIBER PRICE 0.00 -4.68

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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Apr 13, 2007 (20070413/UP).

=> fil reg  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 1.38 381.50  
  
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL  
ENTRY SESSION  
CA SUBSCRIBER PRICE 0.00 -4.68

FILE 'REGISTRY' ENTERED AT 17:03:32 ON 17 APR 2007  
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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 16 APR 2007 HIGHEST RN 930395-50-9  
DICTIONARY FILE UPDATES: 16 APR 2007 HIGHEST RN 930395-50-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

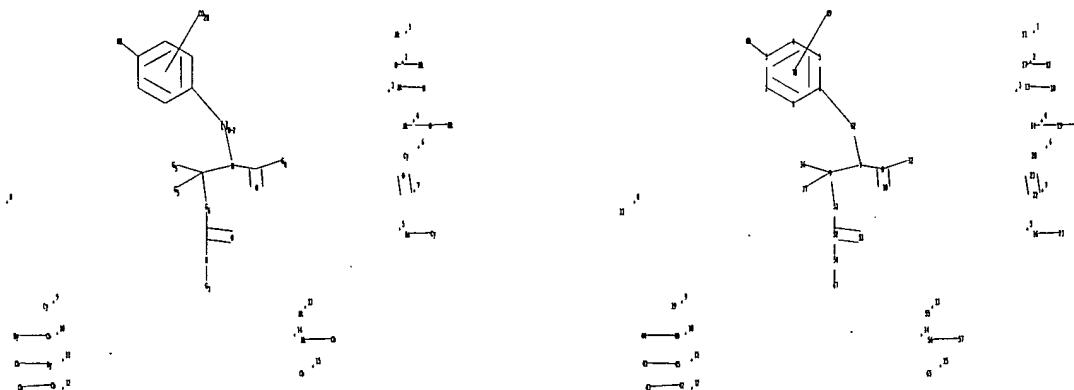
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10565557-formula(IA).str



chain nodes :

7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 32 33 36 37  
39 40 41 42 43 44 45 51 52 53 54 55 56 57 62 65 67 68 69

ring nodes :

1 2 3 4 5 6

chain bonds :

3-68 6-62 7-9 7-8 7-62 8-10 8-32 9-36 9-37 9-51 12-17 13-18 14-19 15-19  
16-21 22-23 40-44 41-45 42-43 51-52 52-53 52-54 54-67 56-57

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

3-68 7-9 7-8 7-62 8-10 8-32 9-36 9-37 9-51 12-17 13-18 14-19 15-19  
16-21

22-23 40-44 41-45 51-52 52-53 52-54 54-67 56-57  
exact bonds :  
6-62 42-43  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

G4:[\*1], [\*2], [\*3], [\*4], [\*5], [\*6], [\*7]

G5:H, [\*8]

G6:[\*9], [\*10], [\*11], [\*12]

G7:[\*13], [\*14], [\*15]

G8:H,CH3

Match level :

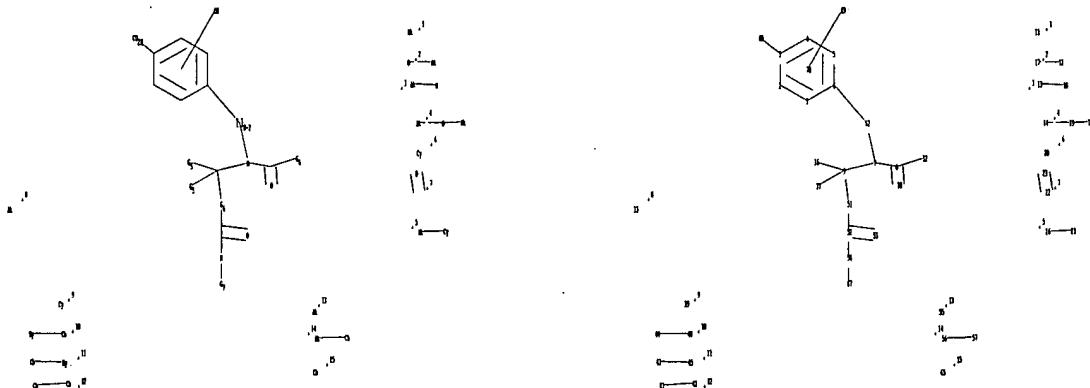
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:Atom  
21:Atom 22:CLASS 23:CLASS 32:CLASS 33:CLASS 36:CLASS 37:CLASS 39:Atom  
40:Atom 41:Atom  
42:Atom 43:Atom 44:Atom 45:Atom 51:CLASS 52:CLASS 53:CLASS 54:CLASS  
55:CLASS 56:CLASS 57:Atom  
62:CLASS 65:Atom 67:CLASS 68:CLASS 69:CLASS 70:Atom

Generic attributes :

33:  
Saturation : Saturated  
40:  
Saturation : Unsaturated  
41:  
Saturation : Unsaturated  
42:  
Saturation : Unsaturated  
43:  
Saturation : Unsaturated  
44:  
Saturation : Unsaturated  
45:  
Saturation : Unsaturated  
57:  
Type of Ring System : Monocyclic

L10 STRUCTURE UPLOADED

=>  
Uploading C:\Program Files\Stnexp\Queries\10565557-formula(IB).str



chain nodes :

7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 32 33 36 37  
39 40 41 42 43 44 45 51 52 53 54 55 56 57 62 65 67 68 69

ring nodes :

1 2 3 4 5 6

chain bonds :

3-68 6-62 7-9 7-8 7-62 8-10 8-32 9-36 9-37 9-51 12-17 13-18 14-19 15-19  
16-21 22-23 40-44 41-45 42-43 51-52 52-53 52-54 54-67 56-57

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

7-9 7-8 7-62 8-10 8-32 9-36 9-37 9-51 12-17 13-18 14-19 15-19 16-21  
22-23 40-44 41-45 51-52 52-53 52-54 54-67 56-57

exact bonds :

3-68 6-62 42-43

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G4: [\*1], [\*2], [\*3], [\*4], [\*5], [\*6], [\*7]

G5:H, [\*8]

G6: [\*9], [\*10], [\*11], [\*12]

G7: [\*13], [\*14], [\*15]

G8:H, CH3

Match level :

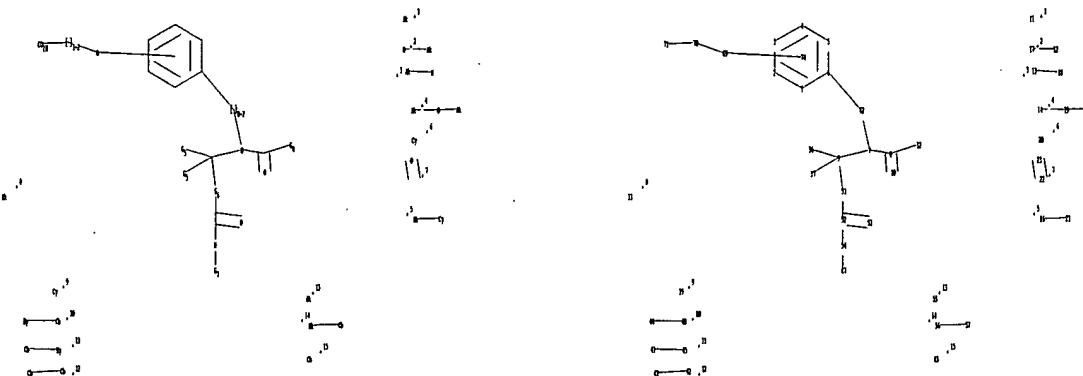
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:Atom  
21:Atom 22:CLASS 23:CLASS 32:CLASS 33:CLASS 36:CLASS 37:CLASS 39:Atom  
40:Atom 41:Atom  
42:Atom 43:Atom 44:Atom 45:Atom 51:CLASS 52:CLASS 53:CLASS 54:CLASS  
55:CLASS 56:CLASS 57:Atom  
62:CLASS 65:Atom 67:CLASS 68:CLASS 69:CLASS 70:Atom

Generic attributes :

33:  
Saturation : Saturated  
40:  
Saturation : Unsaturated  
41:  
Saturation : Unsaturated  
42:  
Saturation : Unsaturated  
43:  
Saturation : Unsaturated  
44:  
Saturation : Unsaturated  
45:  
Saturation : Unsaturated  
57:  
Type of Ring System : Monocyclic

L11 STRUCTURE UPLOADED

=>  
Uploading C:\Program Files\Stnexp\Queries\10565557-formula(IC).str



chain nodes :

7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 32 33 36 37  
39 40 41 42 43 44 45 51 52 53 54 55 56 57 62 65 67 69 70 71

ring nodes :

1 2 3 4 5 6

chain bonds :

6-62 7-9 7-8 7-62 8-10 8-32 9-36 9-37 9-51 12-17 13-18 14-19 15-19  
16-21

22-23 40-44 41-45 42-43 51-52 52-53 52-54 54-67 56-57 69-70 70-71

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

7-9 7-8 7-62 8-10 8-32 9-36 9-37 9-51 12-17 13-18 14-19 15-19 16-21  
22-23 40-44 41-45 51-52 52-53 52-54 54-67 56-57 69-70

exact bonds :

6-62 42-43 70-71

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G4:[\*1], [\*2], [\*3], [\*4], [\*5], [\*6], [\*7]

G5:H, [\*8]

G6:[\*9], [\*10], [\*11], [\*12]

G7:[\*13], [\*14], [\*15]

G8:H, CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS  
19:CLASS 20:Atom  
21:Atom 22:CLASS 23:CLASS 32:CLASS 33:CLASS 36:CLASS 37:CLASS 39:Atom  
40:Atom 41:Atom  
42:Atom 43:Atom 44:Atom 45:Atom 51:CLASS 52:CLASS 53:CLASS 54:CLASS  
55:CLASS 56:CLASS 57:Atom  
62:CLASS 65:Atom 67:CLASS 69:CLASS 70:CLASS 71:CLASS 74:Atom

Generic attributes :

33:  
Saturation : Saturated  
40:  
Saturation : Unsaturated  
41:  
Saturation : Unsaturated  
42:  
Saturation : Unsaturated  
43:  
Saturation : Unsaturated  
44:  
Saturation : Unsaturated  
45:  
Saturation : Unsaturated  
57:  
Type of Ring System : Monocyclic

L12 STRUCTURE UPLOADED

=> d his

(FILE 'HOME' ENTERED AT 16:20:09 ON 17 APR 2007)

FILE 'REGISTRY' ENTERED AT 16:20:17 ON 17 APR 2007

L1 STRUCTURE UPLOADED  
L2 0 S L1  
L3 STRUCTURE UPLOADED  
L4 1 S L3  
L5 35 S L3 SSS FULL  
SAV TEM BRD565557/A L5

FILE 'CAPLUS' ENTERED AT 16:24:21 ON 17 APR 2007

L6 6 S L5  
SAV TEM ANS565557/A L6

FILE 'REGISTRY' ENTERED AT 16:48:34 ON 17 APR 2007

L7 STRUCTURE UPLOADED  
L8 9 S L7  
L9 855 S L7 SSS FULL  
SAV TEM BRI565557/A L9

FILE 'STNGUIDE' ENTERED AT 16:49:43 ON 17 APR 2007

FILE 'REGISTRY' ENTERED AT 17:03:32 ON 17 APR 2007

L10 STRUCTURE UPLOADED  
L11 STRUCTURE UPLOADED  
L12 STRUCTURE UPLOADED

=> s 110 sub=19 sss full

FULL SUBSET SEARCH INITIATED 17:04:59 FILE 'REGISTRY'  
FULL SUBSET SCREEN SEARCH COMPLETED - 60 TO ITERATE

100.0% PROCESSED 60 ITERATIONS 28 ANSWERS  
SEARCH TIME: 00.00.01

L13 28 SEA SUB=L9 SSS FUL L10

=> sav tem FIA565557/a 113

=> s 111 sub=19 sss full  
FULL SUBSET SEARCH INITIATED 17:05:31 FILE 'REGISTRY'  
FULL SUBSET SCREEN SEARCH COMPLETED - 115 TO ITERATE

100.0% PROCESSED 115 ITERATIONS 2 ANSWERS  
SEARCH TIME: 00.00.01

L14 2 SEA SUB=L9 SSS FUL L11

=> sav tem FIB565557/a 114

=> s 112 sub=19 sss full  
FULL SUBSET SEARCH INITIATED 17:06:05 FILE 'REGISTRY'  
FULL SUBSET SCREEN SEARCH COMPLETED - 92 TO ITERATE

100.0% PROCESSED 92 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

L15 1 SEA SUB=L9 SSS FUL L12

=> sav tem FIC565557/a 115

=> fil caplus			
COST IN U.S. DOLLARS	SINCE FILE	TOTAL	
	ENTRY	SESSION	
FULL ESTIMATED COST	124.20	505.70	
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL	
	ENTRY	SESSION	
CA SUBSCRIBER PRICE	0.00	-4.68	

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FILE COVERS 1907 - 17 Apr 2007 VOL 146 ISS 17  
FILE LAST UPDATED: 15 Apr 2007 (20070415/ED)

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=> d his

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FILE 'REGISTRY' ENTERED AT 16:20:17 ON 17 APR 2007

L1                   STRUCTURE uploaded  
L2                   0 S L1  
L3                   STRUCTURE uploaded  
L4                   1 S L3  
L5                   35 S L3 SSS FULL  
                      SAV TEM BRD565557/A L5

FILE 'CAPLUS' ENTERED AT 16:24:21 ON 17 APR 2007

L6                   6 S L5  
                      SAV TEM ANS565557/A L6

FILE 'REGISTRY' ENTERED AT 16:48:34 ON 17 APR 2007

L7                   STRUCTURE uploaded  
L8                   9 S L7  
L9                   855 S L7 SSS FULL  
                      SAV TEM BRI565557/A L9

FILE 'STNGUIDE' ENTERED AT 16:49:43 ON 17 APR 2007

FILE 'REGISTRY' ENTERED AT 17:03:32 ON 17 APR 2007

L10                  STRUCTURE uploaded  
L11                  STRUCTURE uploaded  
L12                  STRUCTURE uploaded  
L13                  28 S L10 SSS FULL SUB=L9  
                      SAV TEM FIA565557/A L13  
L14                  2 S L11 SSS FULL SUB=L9  
                      SAV TEM FIB565557/A L14  
L15                  1 S L12 SSS FULL SUB=L9  
                      SAV TEM FIC565557/A L15

FILE 'CAPLUS' ENTERED AT 17:06:23 ON 17 APR 2007

=> s l13  
L16                  4 L13

=> s l14  
L17                  1 L14

=> s l15  
L18                  1 L15

=> s l17 not l16  
L19                  0 L17 NOT L16

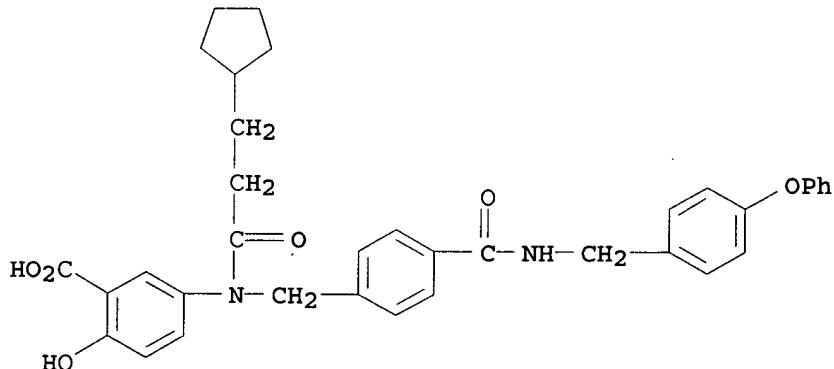
=> s l18 not l16  
L20                  0 L18 NOT L16

=> d l16 bib abs hitstr

L16   ANSWER 1 OF 4   CAPLUS   COPYRIGHT 2007 ACS on STN  
AN   2007:87128   CAPLUS <<LOGINID::20070417>>  
DN   146:177185  
TI   Glepp-1 inhibitors in the treatment of autoimmune and/or inflammatory  
      disorders  
IN   Bombrun, Agnes; Hooft van Huijsduijnen, Rob; Jorand-Lebrun, Catherine;  
      Vitte, Pierre-Alain; Gerber, Patrick  
PA   Applied Research Systems Ars Holding N. V., Neth. Antilles  
SO   PCT Int. Appl., 77pp.

CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2007009959	A1	20070125	WO 2006-EP64288	20060714
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
PRAI	EP 2005-106547	A	20050715		
	US 2005-706365P	P	20050808		
OS	MARPAT 146:177185				
AB	The present invention is related to the use of a Glepp-1 inhibitor for the manufacture of a medicament for the treatment of an autoimmune and/or an inflammatory disorder.				
IT	842136-75-8				
	RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (Glepp-1 inhibitors in treatment of autoimmune and/or inflammatory disorders)				
RN	842136-75-8 CAPLUS				
CN	Benzoic acid, 5-[(3-cyclopentyl-1-oxopropyl)[[4-[[[(4-phenoxyphenyl)methyl]amino]carbonyl]phenyl]methyl]amino]-2-hydroxy- (9CI) (CA INDEX NAME)				



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log hold  
 COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE  
 ENTRY

6.21 511.91

SINCE FILE  
 ENTRY

-0.78 -5.46

SESSION WILL BE HELD FOR 120 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 17:07:40 ON 17 APR 2007

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptasj11626

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'CAPLUS' AT 17:14:08 ON 17 APR 2007  
FILE 'CAPLUS' ENTERED AT 17:14:08 ON 17 APR 2007  
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	6.21	511.91
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.78	-5.46

=> d his

(FILE 'HOME' ENTERED AT 16:20:09 ON 17 APR 2007)

FILE 'REGISTRY' ENTERED AT 16:20:17 ON 17 APR 2007

L1           STRUCTURE UPLOADED  
L2           0 S L1  
L3           STRUCTURE UPLOADED  
L4           1 S L3  
L5           35 S L3 SSS FULL  
              SAV TEM BRD565557/A L5

FILE 'CAPLUS' ENTERED AT 16:24:21 ON 17 APR 2007

L6           6 S L5  
              SAV TEM ANS565557/A L6

FILE 'REGISTRY' ENTERED AT 16:48:34 ON 17 APR 2007

L7           STRUCTURE UPLOADED  
L8           9 S L7  
L9           855 S L7 SSS FULL  
              SAV TEM BRI565557/A L9

FILE 'STNGUIDE' ENTERED AT 16:49:43 ON 17 APR 2007

FILE 'REGISTRY' ENTERED AT 17:03:32 ON 17 APR 2007

L10          STRUCTURE UPLOADED  
L11          STRUCTURE UPLOADED  
L12          STRUCTURE UPLOADED  
L13          28 S L10 SSS FULL SUB=L9  
              SAV TEM FIA565557/A L13  
L14          2 S L11 SSS FULL SUB=L9  
              SAV TEM FIB565557/A L14  
L15          1 S L12 SSS FULL SUB=L9  
              SAV TEM FIC565557/A L15

FILE 'CAPLUS' ENTERED AT 17:06:23 ON 17 APR 2007

L16          4 S L13

L17 1 S L14  
L18 1 S L15  
L19 0 S L17 NOT L16  
L20 0 S L18 NOT L16

=> log off

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:y

STN INTERNATIONAL LOGOFF AT 17:14:23 ON 17 APR 2007